



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:00 AM UTC

PDB ID : 3CHX / pdb_00003chx
Title : Crystal structure of Methylosinus trichosporium OB3b particulate methane monooxygenase (pMMO)
Authors : Hakemian, A.S.
Deposited on : 2008-03-10
Resolution : 3.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

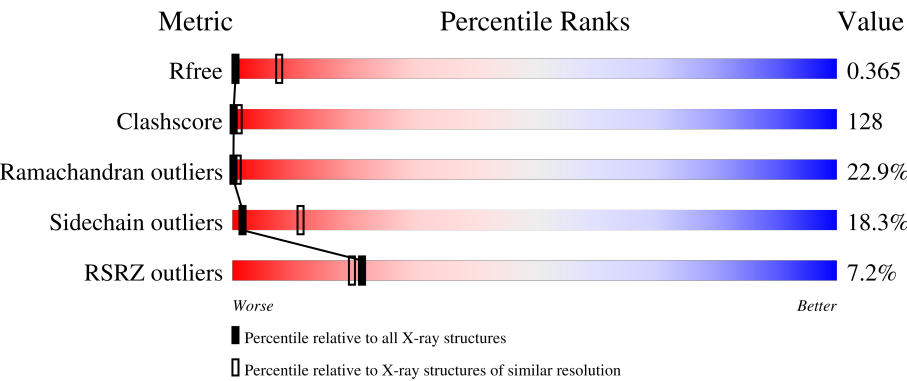
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1270 (4.10-3.70)
Clashscore	190562	1034 (4.08-3.72)
Ramachandran outliers	187476	1251 (4.10-3.70)
Sidechain outliers	187428	1243 (4.10-3.70)
RSRZ outliers	180081	1269 (4.10-3.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	392	6% 8%55%26%8%
1	E	392	3% 8%55%26%8%
1	I	392	5% 8%56%26%8%
2	B	252	7% 42%36%12%6%
2	F	252	10% 5%42%36%12%6%

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Mol	Chain	Length	Quality of chain
2	J	252	10% 43% 36% 12% 6%
3	C	256	5% 34% 21% 38%
3	G	256	5% 34% 21% 38%
3	K	256	5% 34% 20% 38%
4	D	20	40% 60%
4	H	20	40% 60%
4	L	20	40% 60%
5	M	26	19% 81%
5	N	26	19% 81%
5	O	26	19% 81%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 18945 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called PmoB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	362	Total	C	N	O	S	0	0	0
			2832	1831	478	518	5			
1	E	362	Total	C	N	O	S	0	0	0
			2832	1831	478	518	5			
1	I	362	Total	C	N	O	S	0	0	0
			2832	1831	478	518	5			

- Molecule 2 is a protein called PmoA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	238	Total	C	N	O	S	0	0	0
			1925	1303	301	310	11			
2	F	238	Total	C	N	O	S	0	0	0
			1925	1303	301	310	11			
2	J	238	Total	C	N	O	S	0	0	0
			1925	1303	301	310	11			

- Molecule 3 is a protein called PmoC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	159	Total	C	N	O	S	0	0	0
			1324	886	211	223	4			
3	G	159	Total	C	N	O	S	0	0	0
			1324	886	211	223	4			
3	K	159	Total	C	N	O	S	0	0	0
			1324	886	211	223	4			

- Molecule 4 is a protein called 20-residue peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	20	Total	C	N	O	0	0	0
			100	60	20	20			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	H	20	Total	C	N	O	0	0	0
			100	60	20	20			
4	L	20	Total	C	N	O	0	0	0
			100	60	20	20			

- Molecule 5 is a protein called 26-residue peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	M	26	Total	C	N	O	0	0	0
			131	78	26	27			
5	N	26	Total	C	N	O	0	0	0
			131	78	26	27			
5	O	26	Total	C	N	O	0	0	0
			131	78	26	27			

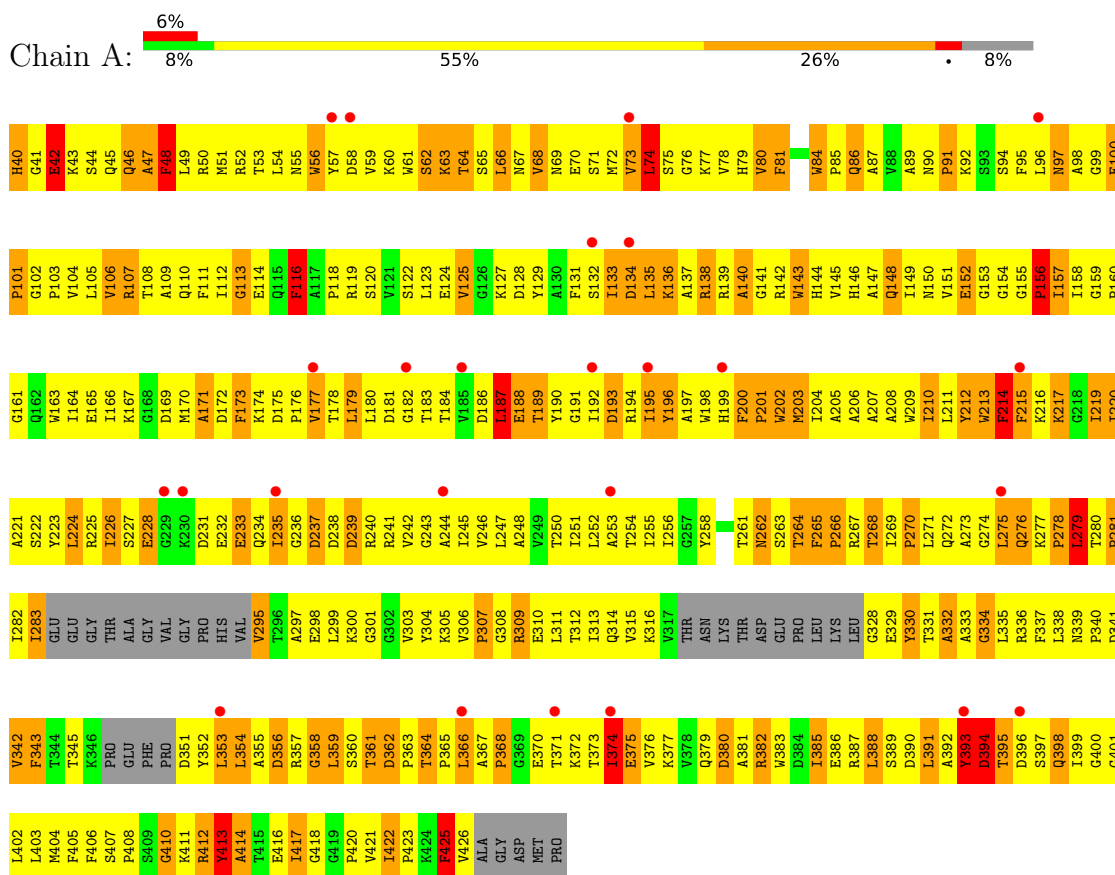
- Molecule 6 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	Cu	0	0
			2	2		
6	C	1	Total	Cu	0	0
			1	1		
6	E	2	Total	Cu	0	0
			2	2		
6	G	1	Total	Cu	0	0
			1	1		
6	I	2	Total	Cu	0	0
			2	2		
6	K	1	Total	Cu	0	0
			1	1		

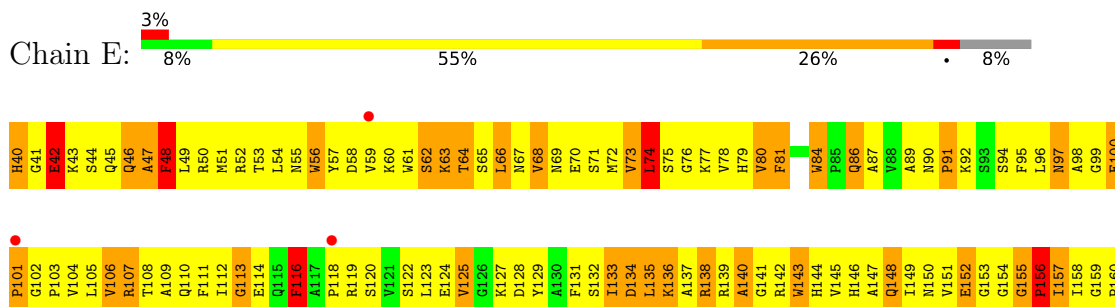
3 Residue-property plots

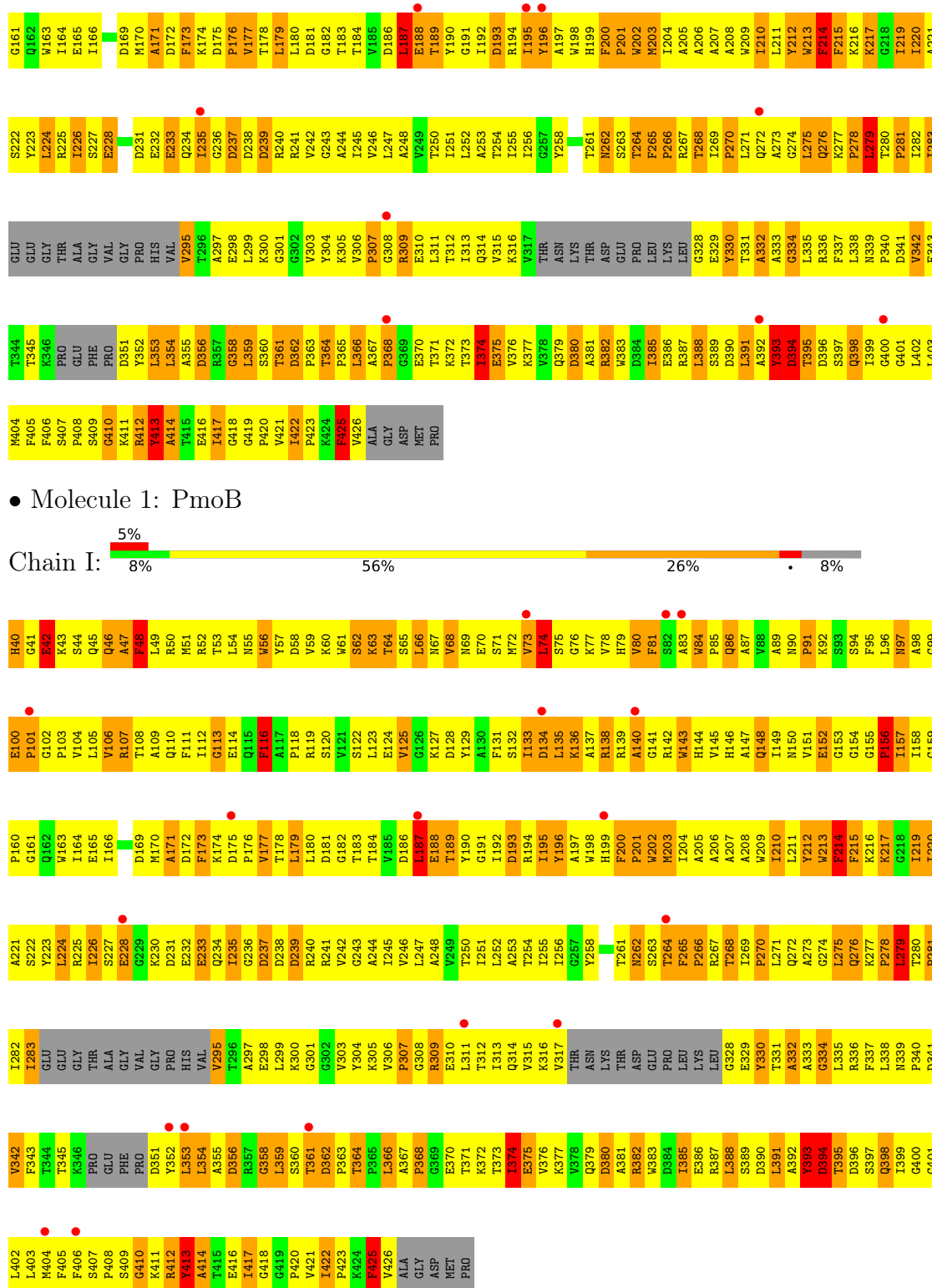
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: PmoB



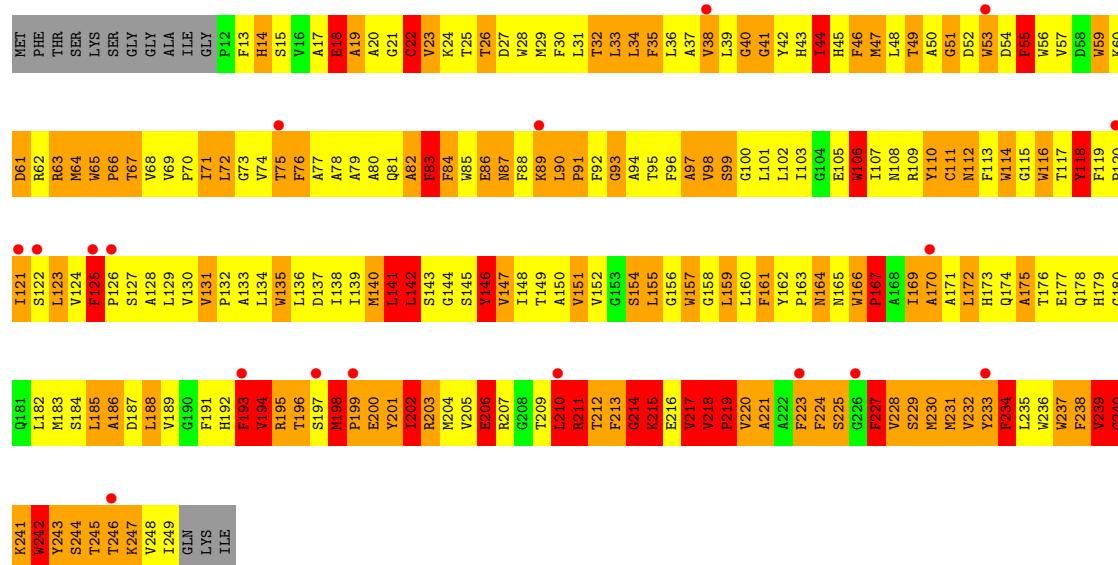
• Molecule 1: PmoB



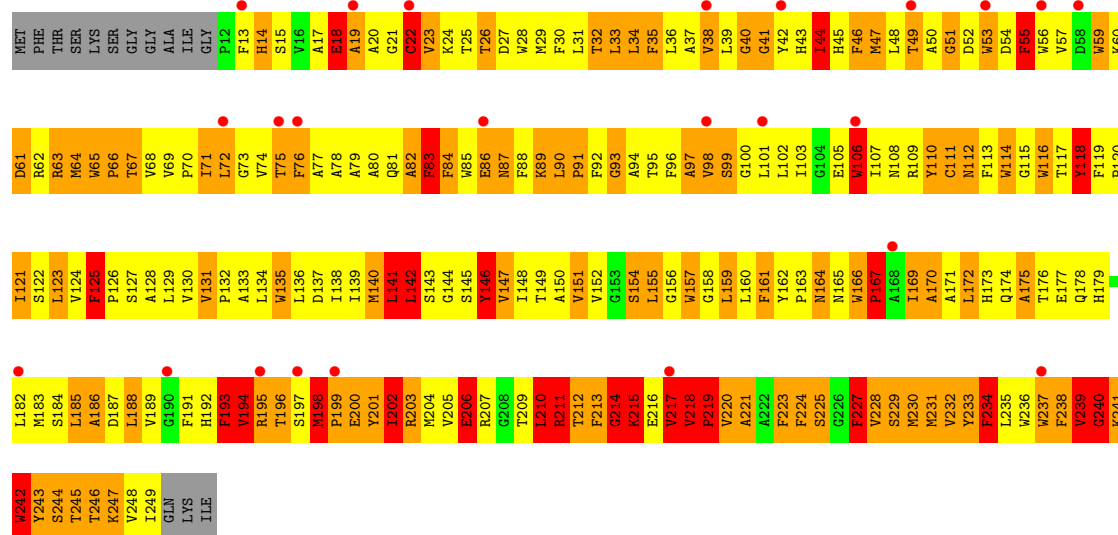


• Molecule 2: PmoA

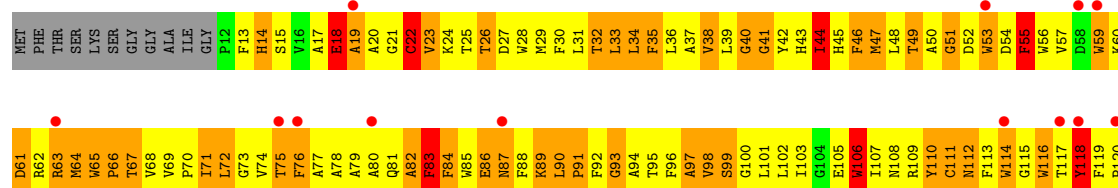


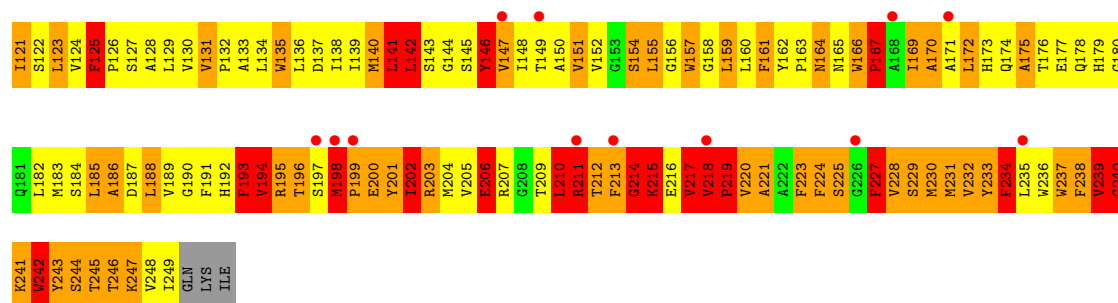


• Molecule 2: PmoA

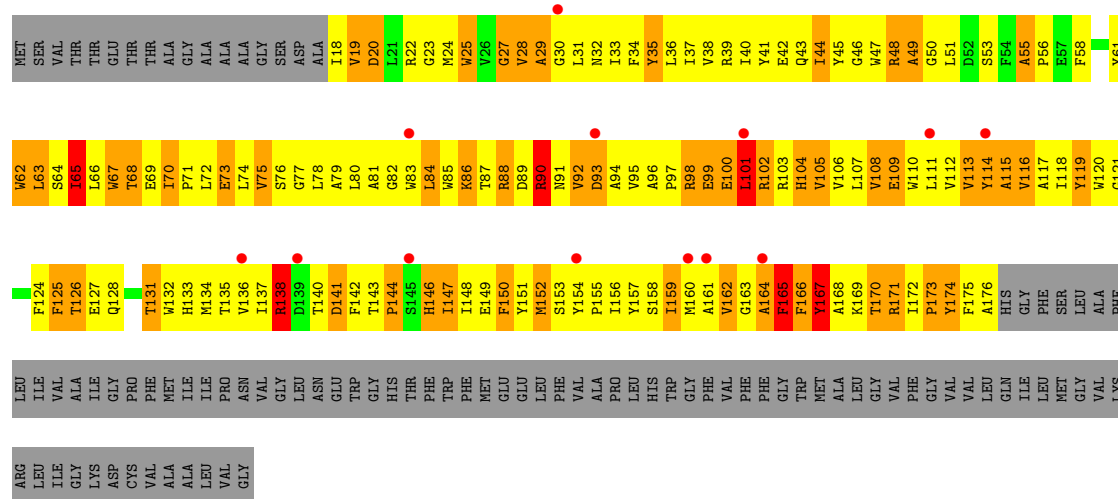


• Molecule 2: PmoA

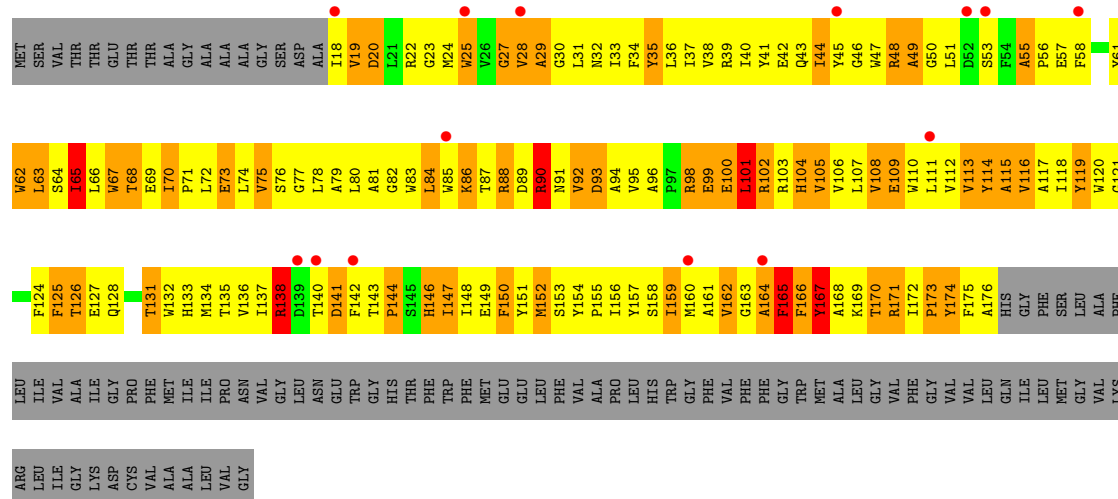




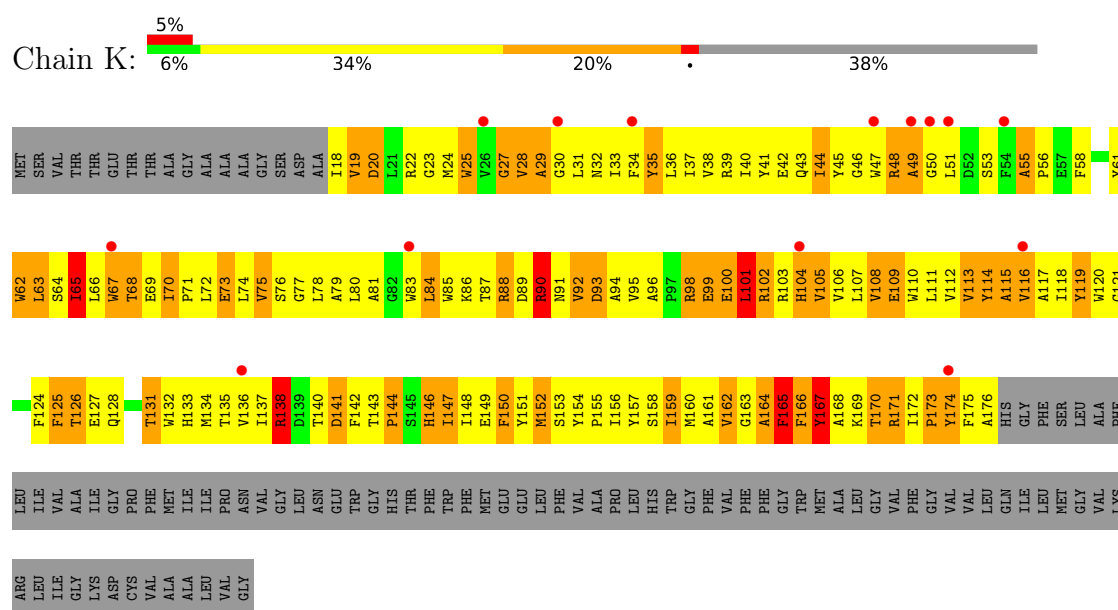
• Molecule 3: PmoC



• Molecule 3: PmoC



• Molecule 3: PmoC



- Molecule 4: 20-residue peptide



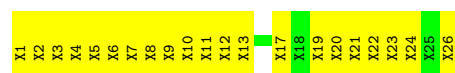
- Molecule 4: 20-residue peptide



- Molecule 4: 20-residue peptide

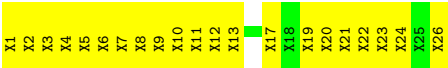


- Molecule 5: 26-residue peptide

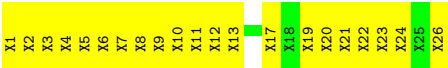


- Molecule 5: 26-residue peptide





● Molecule 5: 26-residue peptide



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	113.81Å 184.07Å 203.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.00 – 3.90 38.00 – 3.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (38.00-3.90) 99.8 (38.00-3.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.84 (at 3.87Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.342 , 0.377 0.331 , 0.365	Depositor DCC
R_{free} test set	3992 reflections (10.06%)	wwPDB-VP
Wilson B-factor (Å ²)	121.3	Xtriage
Anisotropy	0.991	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 115.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	18945	wwPDB-VP
Average B, all atoms (Å ²)	141.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.82% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CU

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.56	0/2902	1.25	36/3944 (0.9%)
1	E	0.56	0/2902	1.25	36/3944 (0.9%)
1	I	0.56	0/2902	1.25	36/3944 (0.9%)
2	B	0.71	2/2002 (0.1%)	1.35	35/2740 (1.3%)
2	F	0.71	2/2002 (0.1%)	1.35	35/2740 (1.3%)
2	J	0.71	2/2002 (0.1%)	1.35	35/2740 (1.3%)
3	C	0.57	0/1371	1.13	16/1876 (0.9%)
3	G	0.57	0/1371	1.13	16/1876 (0.9%)
3	K	0.57	0/1371	1.13	16/1876 (0.9%)
All	All	0.62	6/18825 (0.0%)	1.26	261/25680 (1.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	197	SER	CA-C	6.50	1.57	1.53
2	B	197	SER	CA-C	6.49	1.57	1.53
2	F	197	SER	CA-C	6.37	1.57	1.53
2	J	197	SER	N-CA	5.99	1.50	1.46
2	F	197	SER	N-CA	5.91	1.49	1.46
2	B	197	SER	N-CA	5.85	1.49	1.46

All (261) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	53	TRP	N-CA-C	-17.32	90.10	113.30
2	B	53	TRP	N-CA-C	-17.28	90.14	113.30
2	F	53	TRP	N-CA-C	-17.25	90.19	113.30
2	F	197	SER	N-CA-C	15.18	121.23	108.78
2	J	197	SER	N-CA-C	15.17	121.22	108.78
2	B	197	SER	N-CA-C	15.17	121.22	108.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	247	LYS	N-CA-C	-14.71	92.79	110.44
2	B	247	LYS	N-CA-C	-14.69	92.81	110.44
2	J	247	LYS	N-CA-C	-14.66	92.84	110.44
1	E	203	MET	N-CA-C	-12.48	98.34	113.19
1	A	203	MET	N-CA-C	-12.48	98.34	113.19
1	I	203	MET	N-CA-C	-12.44	98.39	113.19
2	B	238	PHE	N-CA-C	-11.84	101.12	114.62
2	F	238	PHE	N-CA-C	-11.84	101.12	114.62
2	J	238	PHE	N-CA-C	-11.84	101.12	114.62
2	F	225	SER	N-CA-C	11.58	124.20	107.88
2	J	225	SER	N-CA-C	11.56	124.19	107.88
2	B	225	SER	N-CA-C	11.56	124.18	107.88
1	E	202	TRP	N-CA-C	-11.40	101.62	114.62
1	I	202	TRP	N-CA-C	-11.37	101.66	114.62
1	A	202	TRP	N-CA-C	-11.36	101.67	114.62
3	C	23	GLY	N-CA-C	-11.23	100.61	115.32
3	G	23	GLY	N-CA-C	-11.23	100.61	115.32
3	K	23	GLY	N-CA-C	-11.22	100.63	115.32
2	J	227	PHE	N-CA-C	-11.13	99.22	112.92
2	B	227	PHE	N-CA-C	-11.13	99.23	112.92
2	F	227	PHE	N-CA-C	-11.11	99.25	112.92
1	I	264	THR	N-CA-C	-9.74	99.47	112.72
1	A	264	THR	N-CA-C	-9.73	99.48	112.72
1	E	264	THR	N-CA-C	-9.72	99.49	112.72
1	I	97	ASN	N-CA-C	9.66	121.50	107.88
1	A	97	ASN	N-CA-C	9.64	121.48	107.88
1	E	97	ASN	N-CA-C	9.64	121.47	107.88
1	A	334	GLY	N-CA-C	-9.25	103.36	115.47
1	I	334	GLY	N-CA-C	-9.24	103.37	115.47
2	J	38	VAL	N-CA-C	-9.24	101.85	110.53
2	F	38	VAL	N-CA-C	-9.22	101.87	110.53
2	B	38	VAL	N-CA-C	-9.21	101.87	110.53
1	E	334	GLY	N-CA-C	-9.21	103.40	115.47
3	K	67	TRP	N-CA-C	-8.97	102.47	113.15
2	B	243	TYR	N-CA-C	-8.96	100.77	112.68
2	J	243	TYR	N-CA-C	-8.96	100.77	112.68
2	F	243	TYR	N-CA-C	-8.95	100.77	112.68
3	G	67	TRP	N-CA-C	-8.93	102.53	113.15
3	C	67	TRP	N-CA-C	-8.93	102.53	113.15
3	K	113	VAL	N-CA-C	-8.90	102.19	110.82
3	G	113	VAL	N-CA-C	-8.88	102.20	110.82
1	I	362	ASP	N-CA-C	-8.87	92.16	109.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	362	ASP	N-CA-C	-8.86	92.17	109.10
3	C	113	VAL	N-CA-C	-8.86	102.22	110.82
1	E	362	ASP	N-CA-C	-8.86	92.18	109.10
1	A	214	PHE	N-CA-C	-8.84	99.23	113.19
1	E	214	PHE	N-CA-C	-8.84	99.23	113.19
1	I	214	PHE	N-CA-C	-8.82	99.25	113.19
2	F	61	ASP	N-CA-C	8.81	117.21	108.75
2	B	61	ASP	N-CA-C	8.80	117.19	108.75
2	J	61	ASP	N-CA-C	8.79	117.19	108.75
1	I	413	TYR	N-CA-C	-8.59	96.10	109.76
1	A	413	TYR	N-CA-C	-8.58	96.12	109.76
1	E	413	TYR	N-CA-C	-8.56	96.15	109.76
1	E	343	PHE	N-CA-C	8.44	123.22	110.14
1	A	343	PHE	N-CA-C	8.42	123.20	110.14
1	I	343	PHE	N-CA-C	8.38	123.13	110.14
2	F	242	TRP	N-CA-C	-8.10	103.40	113.20
2	B	242	TRP	N-CA-C	-8.08	103.42	113.20
2	J	242	TRP	N-CA-C	-8.08	103.42	113.20
1	I	262	ASN	N-CA-C	-7.67	103.48	112.92
1	E	262	ASN	N-CA-C	-7.67	103.49	112.92
1	A	262	ASN	N-CA-C	-7.66	103.49	112.92
2	F	20	ALA	N-CA-C	-7.66	104.07	113.41
2	J	20	ALA	N-CA-C	-7.66	104.07	113.41
2	B	20	ALA	N-CA-C	-7.64	104.08	113.41
1	A	224	LEU	N-CA-C	-7.60	102.97	111.71
1	I	224	LEU	N-CA-C	-7.60	102.97	111.71
1	E	224	LEU	N-CA-C	-7.59	102.98	111.71
2	B	67	THR	N-CA-C	-7.56	104.96	114.56
2	F	67	THR	N-CA-C	-7.56	104.96	114.56
2	J	67	THR	N-CA-C	-7.56	104.96	114.56
2	J	241	LYS	N-CA-C	-7.48	103.21	111.36
2	F	241	LYS	N-CA-C	-7.47	103.22	111.36
2	B	241	LYS	N-CA-C	-7.46	103.23	111.36
3	C	141	ASP	N-CA-C	-7.26	104.86	113.21
3	G	141	ASP	N-CA-C	-7.25	104.87	113.21
3	K	141	ASP	N-CA-C	-7.24	104.88	113.21
1	E	412	ARG	N-CA-C	7.20	126.14	110.80
1	A	412	ARG	N-CA-C	7.18	126.10	110.80
1	I	364	THR	CA-C-N	7.18	126.94	119.76
1	I	364	THR	C-N-CA	7.18	126.94	119.76
1	I	412	ARG	N-CA-C	7.18	126.08	110.80
1	A	364	THR	CA-C-N	7.17	126.93	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	364	THR	C-N-CA	7.17	126.93	119.76
1	E	364	THR	CA-C-N	7.13	126.89	119.76
1	E	364	THR	C-N-CA	7.13	126.89	119.76
2	J	218	VAL	N-CA-C	-7.03	93.69	108.88
2	B	218	VAL	N-CA-C	-7.01	93.74	108.88
2	F	218	VAL	N-CA-C	-7.00	93.75	108.88
2	B	59	TRP	N-CA-C	-6.88	104.91	113.38
2	J	59	TRP	N-CA-C	-6.88	104.92	113.38
2	F	59	TRP	N-CA-C	-6.86	104.94	113.38
2	B	218	VAL	C-N-CD	-6.70	105.86	120.60
2	F	218	VAL	C-N-CD	-6.70	105.86	120.60
1	I	133	ILE	N-CA-C	6.70	117.76	107.78
2	J	218	VAL	C-N-CD	-6.69	105.88	120.60
1	A	133	ILE	N-CA-C	6.68	117.74	107.78
1	E	133	ILE	N-CA-C	6.67	117.72	107.78
2	J	154	SER	N-CA-C	-6.64	103.96	111.07
2	F	154	SER	N-CA-C	-6.63	103.97	111.07
3	C	104	HIS	N-CA-C	-6.61	103.89	112.68
2	B	154	SER	N-CA-C	-6.61	104.00	111.07
3	K	104	HIS	N-CA-C	-6.61	103.89	112.68
3	C	109	GLU	N-CA-C	-6.59	104.16	112.93
3	G	104	HIS	N-CA-C	-6.59	103.91	112.68
3	K	109	GLU	N-CA-C	-6.59	104.16	112.93
2	F	185	LEU	N-CA-C	-6.59	100.50	111.37
3	G	109	GLU	N-CA-C	-6.58	104.17	112.93
2	B	185	LEU	N-CA-C	-6.58	100.51	111.37
2	J	185	LEU	N-CA-C	-6.58	100.51	111.37
2	B	231	MET	N-CA-C	-6.58	105.41	113.50
2	J	231	MET	N-CA-C	-6.58	105.41	113.50
2	F	231	MET	N-CA-C	-6.55	105.44	113.50
1	E	215	PHE	N-CA-C	-6.48	102.71	112.04
1	I	215	PHE	N-CA-C	-6.47	102.72	112.04
1	A	215	PHE	N-CA-C	-6.46	102.73	112.04
1	E	345	THR	N-CA-C	6.46	124.55	110.80
1	A	345	THR	N-CA-C	6.45	124.55	110.80
1	I	345	THR	N-CA-C	6.42	124.48	110.80
1	E	113	GLY	N-CA-C	-6.41	100.64	111.73
1	E	187	LEU	N-CA-C	6.40	118.14	111.03
1	A	113	GLY	N-CA-C	-6.40	100.66	111.73
1	I	113	GLY	N-CA-C	-6.40	100.66	111.73
1	A	187	LEU	N-CA-C	6.38	118.11	111.03
1	I	187	LEU	N-CA-C	6.36	118.08	111.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	240	GLY	N-CA-C	-6.35	98.13	113.18
2	B	240	GLY	N-CA-C	-6.35	98.13	113.18
2	F	240	GLY	N-CA-C	-6.34	98.15	113.18
3	G	131	THR	N-CA-C	-6.28	104.67	112.90
3	C	131	THR	N-CA-C	-6.25	104.71	112.90
3	K	131	THR	N-CA-C	-6.24	104.73	112.90
3	G	75	VAL	N-CA-C	-6.22	104.43	110.72
2	F	211	ARG	N-CA-C	-6.22	104.25	112.34
2	B	211	ARG	N-CA-C	-6.21	104.27	112.34
3	C	75	VAL	N-CA-C	-6.19	104.47	110.72
3	K	75	VAL	N-CA-C	-6.18	104.47	110.72
2	F	142	LEU	N-CA-C	-6.18	101.27	110.23
2	B	214	GLY	N-CA-C	-6.18	98.54	113.18
2	J	142	LEU	N-CA-C	-6.18	101.27	110.23
2	J	19	ALA	N-CA-C	-6.18	104.84	112.38
2	F	214	GLY	N-CA-C	-6.18	98.54	113.18
2	J	214	GLY	N-CA-C	-6.17	98.55	113.18
2	J	211	ARG	N-CA-C	-6.17	104.31	112.34
2	B	142	LEU	N-CA-C	-6.17	101.28	110.23
2	B	19	ALA	N-CA-C	-6.16	104.87	112.38
2	F	19	ALA	N-CA-C	-6.14	104.89	112.38
2	B	26	THR	N-CA-C	-6.12	104.72	111.82
2	B	175	ALA	N-CA-C	6.12	119.17	109.50
2	F	26	THR	N-CA-C	-6.12	104.72	111.82
2	J	175	ALA	N-CA-C	6.12	119.17	109.50
2	F	175	ALA	N-CA-C	6.11	119.15	109.50
2	J	26	THR	N-CA-C	-6.11	104.73	111.82
2	J	194	VAL	N-CA-C	5.99	117.73	109.46
2	B	194	VAL	N-CA-C	5.96	117.69	109.46
2	F	194	VAL	N-CA-C	5.93	117.64	109.46
1	A	330	TYR	N-CA-C	5.88	117.63	107.93
1	E	330	TYR	N-CA-C	5.87	117.61	107.93
1	I	330	TYR	N-CA-C	5.87	117.61	107.93
3	C	98	ARG	N-CA-C	-5.86	104.30	112.45
3	K	98	ARG	N-CA-C	-5.86	104.31	112.45
3	G	98	ARG	N-CA-C	-5.82	104.36	112.45
1	I	425	PHE	N-CA-C	5.78	118.80	109.79
3	K	126	THR	N-CA-C	-5.77	105.91	113.12
1	E	425	PHE	N-CA-C	5.76	118.77	109.79
1	A	425	PHE	N-CA-C	5.75	118.76	109.79
3	G	126	THR	N-CA-C	-5.75	105.94	113.12
3	C	126	THR	N-CA-C	-5.74	105.94	113.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	138	ARG	N-CA-C	-5.70	108.12	114.62
1	A	138	ARG	N-CA-C	-5.70	108.12	114.62
2	F	197	SER	CB-CA-C	-5.69	108.88	117.07
2	B	197	SER	CB-CA-C	-5.69	108.88	117.07
1	I	388	LEU	N-CA-C	-5.68	108.14	114.62
3	K	55	ALA	CA-C-N	5.68	126.94	119.84
3	K	55	ALA	C-N-CA	5.68	126.94	119.84
1	E	138	ARG	N-CA-C	-5.67	108.15	114.62
2	J	197	SER	CB-CA-C	-5.67	108.90	117.07
1	A	388	LEU	N-CA-C	-5.67	108.16	114.62
3	C	165	PHE	N-CA-C	-5.67	98.72	110.80
3	G	165	PHE	N-CA-C	-5.67	98.73	110.80
3	K	165	PHE	N-CA-C	-5.67	98.73	110.80
1	E	388	LEU	N-CA-C	-5.66	108.17	114.62
3	G	55	ALA	CA-C-N	5.66	126.91	119.84
3	G	55	ALA	C-N-CA	5.66	126.91	119.84
3	C	114	TYR	N-CA-C	-5.65	104.49	111.33
3	C	55	ALA	CA-C-N	5.65	126.90	119.84
3	C	55	ALA	C-N-CA	5.65	126.90	119.84
3	G	114	TYR	N-CA-C	-5.65	104.50	111.33
1	E	56	TRP	N-CA-C	5.64	118.23	107.75
3	K	114	TYR	N-CA-C	-5.63	104.51	111.33
1	A	56	TRP	N-CA-C	5.63	118.22	107.75
1	I	56	TRP	N-CA-C	5.62	118.21	107.75
2	J	202	ILE	N-CA-C	-5.57	97.76	109.34
2	B	202	ILE	N-CA-C	-5.56	97.77	109.34
2	F	202	ILE	N-CA-C	-5.54	97.81	109.34
1	A	116	PHE	N-CA-C	-5.53	99.72	108.73
1	I	116	PHE	N-CA-C	-5.52	99.74	108.73
1	E	116	PHE	N-CA-C	-5.50	99.76	108.73
1	I	84	TRP	CA-C-N	5.40	126.59	119.84
1	I	84	TRP	C-N-CA	5.40	126.59	119.84
1	A	84	TRP	CA-C-N	5.39	126.57	119.84
1	A	84	TRP	C-N-CA	5.39	126.57	119.84
1	E	84	TRP	CA-C-N	5.38	126.56	119.84
1	E	84	TRP	C-N-CA	5.38	126.56	119.84
2	J	159	LEU	N-CA-C	-5.37	104.67	111.11
1	A	74	LEU	N-CA-C	-5.37	102.34	110.28
1	I	74	LEU	N-CA-C	-5.36	102.34	110.28
1	E	74	LEU	N-CA-C	-5.36	102.35	110.28
1	E	389	SER	N-CA-C	-5.35	105.99	113.37
2	B	159	LEU	N-CA-C	-5.35	104.69	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	20	ASP	N-CA-C	5.35	122.19	110.80
1	A	255	ILE	N-CA-C	-5.34	104.20	111.89
3	C	20	ASP	N-CA-C	5.34	122.17	110.80
1	I	255	ILE	N-CA-C	-5.34	104.20	111.89
1	A	389	SER	N-CA-C	-5.34	106.00	113.37
1	E	255	ILE	N-CA-C	-5.34	104.20	111.89
2	F	159	LEU	N-CA-C	-5.34	104.71	111.11
1	I	389	SER	N-CA-C	-5.33	106.02	113.37
3	G	20	ASP	N-CA-C	5.32	122.14	110.80
3	C	167	TYR	N-CA-C	-5.25	105.20	111.03
3	G	167	TYR	N-CA-C	-5.25	105.20	111.03
3	K	167	TYR	N-CA-C	-5.24	105.21	111.03
2	B	198	MET	C-N-CD	-5.23	109.09	120.60
2	J	198	MET	C-N-CD	-5.22	109.11	120.60
2	F	198	MET	C-N-CD	-5.22	109.12	120.60
1	A	66	LEU	N-CA-C	-5.18	103.69	110.53
1	E	66	LEU	N-CA-C	-5.18	103.69	110.53
1	I	66	LEU	N-CA-C	-5.17	103.71	110.53
1	E	155	GLY	CA-C-N	5.14	126.26	119.84
1	E	155	GLY	C-N-CA	5.14	126.26	119.84
1	I	414	ALA	N-CA-C	5.13	117.26	108.90
1	A	155	GLY	CA-C-N	5.12	126.25	119.84
1	A	155	GLY	C-N-CA	5.12	126.25	119.84
1	I	155	GLY	CA-C-N	5.11	126.22	119.84
1	I	155	GLY	C-N-CA	5.11	126.22	119.84
1	A	414	ALA	N-CA-C	5.10	117.21	108.90
1	E	414	ALA	N-CA-C	5.09	117.20	108.90
1	I	362	ASP	CA-C-N	5.09	126.20	119.84
1	I	362	ASP	C-N-CA	5.09	126.20	119.84
2	F	197	SER	CA-C-O	5.08	120.89	117.94
2	B	197	SER	CA-C-O	5.07	120.88	117.94
1	A	362	ASP	CA-C-N	5.07	126.17	119.84
1	A	362	ASP	C-N-CA	5.07	126.17	119.84
2	J	197	SER	CA-C-O	5.05	120.87	117.94
1	E	362	ASP	CA-C-N	5.05	126.15	119.84
1	E	362	ASP	C-N-CA	5.05	126.15	119.84
2	J	125	PHE	CA-C-N	5.03	126.12	119.84
2	J	125	PHE	C-N-CA	5.03	126.12	119.84
2	F	18	GLU	N-CA-C	-5.02	100.11	110.80
2	B	125	PHE	CA-C-N	5.01	126.10	119.84
2	B	125	PHE	C-N-CA	5.01	126.10	119.84
2	B	18	GLU	N-CA-C	-5.00	100.14	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	125	PHE	CA-C-N	5.00	126.09	119.84
2	F	125	PHE	C-N-CA	5.00	126.09	119.84
2	J	18	GLU	N-CA-C	-5.00	100.14	110.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2832	0	2837	741	1
1	E	2832	0	2837	740	0
1	I	2832	0	2837	746	1
2	B	1925	0	1884	626	0
2	F	1925	0	1884	636	0
2	J	1925	0	1884	642	0
3	C	1324	0	1292	349	0
3	G	1324	0	1292	346	0
3	K	1324	0	1292	343	0
4	D	100	0	22	18	0
4	H	100	0	22	18	0
4	L	100	0	22	19	0
5	M	131	0	28	30	0
5	N	131	0	28	30	0
5	O	131	0	28	30	0
6	A	2	0	0	0	0
6	C	1	0	0	0	0
6	E	2	0	0	0	0
6	G	1	0	0	0	0
6	I	2	0	0	0	0
6	K	1	0	0	0	0
All	All	18945	0	18189	4765	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 128.

All (4765) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:114:GLU:HG3	1:E:280:THR:HB	1.25	1.19
1:E:309:ARG:HD2	1:E:381:ALA:HA	1.22	1.16
1:I:359:LEU:HD21	1:I:376:VAL:HG13	1.17	1.15
1:A:359:LEU:HD21	1:A:376:VAL:HG13	1.17	1.15
1:A:309:ARG:HD2	1:A:381:ALA:HA	1.22	1.14
1:A:114:GLU:HG3	1:A:280:THR:HB	1.25	1.13
1:A:66:LEU:HD11	1:A:72:MET:HB2	1.28	1.12
1:I:261:THR:HG21	2:J:167:PRO:HA	1.30	1.12
1:I:309:ARG:HD2	1:I:381:ALA:HA	1.22	1.12
1:E:261:THR:HG21	2:F:167:PRO:HA	1.30	1.11
1:A:261:THR:HG21	2:B:167:PRO:HA	1.30	1.10
1:I:213:TRP:HE1	2:J:91:PRO:HG2	1.17	1.10
1:I:114:GLU:HG3	1:I:280:THR:HB	1.25	1.10
3:C:90:ARG:HB2	3:C:90:ARG:HH21	1.16	1.09
2:F:121:ILE:H	2:F:121:ILE:HD12	1.18	1.08
1:I:66:LEU:HD11	1:I:72:MET:HB2	1.28	1.08
1:A:213:TRP:HE1	2:B:91:PRO:HG2	1.17	1.08
3:G:90:ARG:HH21	3:G:90:ARG:HB2	1.16	1.08
2:B:211:ARG:NH2	3:C:158:SER:HA	1.70	1.07
1:E:359:LEU:HD21	1:E:376:VAL:HG13	1.17	1.07
1:E:213:TRP:HE1	2:F:91:PRO:HG2	1.17	1.07
3:K:88:ARG:HB2	3:K:170:THR:HB	1.36	1.07
3:K:90:ARG:HB2	3:K:90:ARG:HH21	1.16	1.07
1:E:66:LEU:HD11	1:E:72:MET:HB2	1.28	1.06
1:E:329:GLU:HG3	1:E:338:LEU:HA	1.38	1.06
2:B:121:ILE:H	2:B:121:ILE:HD12	1.18	1.06
2:F:211:ARG:NH2	3:G:158:SER:HA	1.70	1.06
3:G:88:ARG:HB2	3:G:170:THR:HB	1.36	1.06
3:C:89:ASP:HB3	3:C:92:VAL:HG22	1.36	1.06
2:J:211:ARG:NH2	3:K:158:SER:HA	1.70	1.05
1:I:219:ILE:HD11	2:J:27:ASP:HA	1.37	1.05
3:K:89:ASP:HB3	3:K:92:VAL:HG22	1.36	1.05
1:A:104:VAL:HG21	1:A:143:TRP:HE1	1.21	1.04
1:E:219:ILE:HD11	2:F:27:ASP:HA	1.37	1.04
3:C:88:ARG:HB2	3:C:170:THR:HB	1.36	1.04
3:G:89:ASP:HB3	3:G:92:VAL:HG22	1.36	1.03
1:A:219:ILE:HD11	2:B:27:ASP:HA	1.37	1.02
1:I:104:VAL:HG21	1:I:143:TRP:HE1	1.21	1.01
1:E:104:VAL:HG21	1:E:143:TRP:HE1	1.21	1.01
3:G:88:ARG:HG2	3:G:90:ARG:H	1.24	1.01
1:A:329:GLU:HG3	1:A:338:LEU:HA	1.38	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:121:ILE:H	2:J:121:ILE:HD12	1.18	1.01
1:I:329:GLU:HG3	1:I:338:LEU:HA	1.38	1.01
1:I:179:LEU:HD23	1:I:179:LEU:H	1.27	1.00
1:E:179:LEU:HD23	1:E:179:LEU:H	1.27	0.99
3:C:88:ARG:HG2	3:C:90:ARG:H	1.24	0.99
1:I:192:ILE:HD13	2:J:121:ILE:HD13	1.45	0.98
3:K:88:ARG:HG2	3:K:90:ARG:H	1.24	0.98
1:E:113:GLY:HA3	1:E:279:LEU:HD22	1.45	0.98
2:J:140:MET:HE1	2:J:144:GLY:HA2	1.46	0.98
2:J:244:SER:HA	2:J:247:LYS:HZ2	1.28	0.98
2:F:238:PHE:HB2	2:F:241:LYS:HD2	1.46	0.98
2:B:140:MET:HE1	2:B:144:GLY:HA2	1.46	0.98
2:J:238:PHE:HB2	2:J:241:LYS:HD2	1.46	0.97
1:A:113:GLY:HA3	1:A:279:LEU:HD22	1.45	0.96
2:B:244:SER:HA	2:B:247:LYS:HZ2	1.28	0.96
1:I:113:GLY:HA3	1:I:279:LEU:HD22	1.44	0.96
1:E:192:ILE:HD13	2:F:121:ILE:HD13	1.45	0.96
2:J:102:LEU:HD11	2:J:129:LEU:HD12	1.47	0.96
2:B:203:ARG:HB3	2:B:207:ARG:HH21	1.31	0.96
1:A:192:ILE:HD13	2:B:121:ILE:HD13	1.45	0.96
2:F:140:MET:HE1	2:F:144:GLY:HA2	1.46	0.96
2:F:198:MET:HE2	2:F:198:MET:HA	1.48	0.96
2:F:203:ARG:HB3	2:F:207:ARG:HH21	1.31	0.95
2:J:203:ARG:HB3	2:J:207:ARG:HH21	1.31	0.95
2:B:238:PHE:HB2	2:B:241:LYS:HD2	1.46	0.95
1:A:179:LEU:HD23	1:A:179:LEU:H	1.27	0.95
2:B:102:LEU:HD11	2:B:129:LEU:HD12	1.47	0.94
1:A:52:ARG:HH11	1:A:398:GLN:HB3	1.32	0.94
3:C:172:ILE:HG23	3:C:173:PRO:HD2	1.50	0.94
1:E:114:GLU:CG	1:E:280:THR:HB	1.98	0.94
1:I:119:ARG:HD2	1:I:273:ALA:HA	1.48	0.94
1:A:119:ARG:HD2	1:A:273:ALA:HA	1.48	0.94
3:K:172:ILE:HG23	3:K:173:PRO:HD2	1.50	0.93
2:F:102:LEU:HD11	2:F:129:LEU:HD12	1.47	0.93
1:I:201:PRO:HA	1:I:204:ILE:HD12	1.51	0.93
1:A:66:LEU:HD11	1:A:72:MET:CB	1.98	0.93
1:A:201:PRO:HA	1:A:204:ILE:HD12	1.51	0.93
1:I:52:ARG:HH11	1:I:398:GLN:HB3	1.32	0.93
1:I:66:LEU:HD11	1:I:72:MET:CB	1.98	0.93
1:A:114:GLU:CG	1:A:280:THR:HB	1.98	0.93
1:A:63:LYS:HG3	1:A:64:THR:H	1.34	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:119:ARG:HD2	1:E:273:ALA:HA	1.48	0.92
2:J:198:MET:HE2	2:J:198:MET:HA	1.48	0.92
3:G:172:ILE:HG23	3:G:173:PRO:HD2	1.50	0.92
1:I:114:GLU:CG	1:I:280:THR:HB	1.98	0.92
1:E:66:LEU:HD11	1:E:72:MET:CB	1.98	0.92
1:E:201:PRO:HA	1:E:204:ILE:HD12	1.50	0.92
3:G:162:VAL:O	3:G:166:PHE:HB2	1.69	0.92
1:E:52:ARG:HH11	1:E:398:GLN:HB3	1.32	0.92
1:E:204:ILE:C	1:E:206:ALA:H	1.75	0.92
1:I:204:ILE:C	1:I:206:ALA:H	1.75	0.92
3:K:162:VAL:O	3:K:166:PHE:HB2	1.68	0.92
2:B:239:VAL:O	2:J:205:VAL:HG13	1.69	0.92
2:B:198:MET:HE2	2:B:198:MET:HA	1.48	0.92
1:E:62:SER:HB3	1:E:73:VAL:H	1.35	0.92
1:I:62:SER:HB3	1:I:73:VAL:H	1.35	0.91
2:B:142:LEU:H	2:B:142:LEU:HD12	1.35	0.91
3:C:162:VAL:O	3:C:166:PHE:HB2	1.69	0.91
1:E:329:GLU:HG2	1:E:330:TYR:H	1.34	0.91
1:A:366:LEU:HD12	1:A:370:GLU:OE2	1.71	0.91
1:A:157:ILE:H	1:A:157:ILE:HD12	1.35	0.91
1:E:63:LYS:HG3	1:E:64:THR:H	1.34	0.91
3:C:132:TRP:HE1	3:C:143:THR:HB	1.35	0.91
1:I:157:ILE:H	1:I:157:ILE:HD12	1.35	0.91
3:C:22:ARG:HH12	3:C:25:TRP:HA	1.36	0.90
2:B:82:ALA:HB2	2:B:231:MET:HE2	1.53	0.90
2:B:229:SER:C	2:B:231:MET:H	1.78	0.90
3:G:113:VAL:HB	3:G:160:MET:HE1	1.53	0.90
1:I:63:LYS:HG3	1:I:64:THR:H	1.34	0.90
3:C:138:ARG:NH2	3:C:138:ARG:HB3	1.86	0.90
1:E:105:LEU:HD23	1:E:137:ALA:HA	1.54	0.90
3:C:113:VAL:HB	3:C:160:MET:HE1	1.53	0.90
2:F:82:ALA:HB2	2:F:231:MET:HE2	1.53	0.90
1:I:329:GLU:HG2	1:I:330:TYR:H	1.34	0.90
2:J:229:SER:C	2:J:231:MET:H	1.78	0.90
1:A:204:ILE:C	1:A:206:ALA:H	1.75	0.90
3:G:90:ARG:HB2	3:G:90:ARG:NH2	1.87	0.90
1:I:338:LEU:O	1:I:340:PRO:HD3	1.72	0.90
1:A:269:ILE:HB	1:A:270:PRO:HD2	1.54	0.90
3:K:132:TRP:HE1	3:K:143:THR:HB	1.35	0.90
1:A:105:LEU:HD23	1:A:137:ALA:HA	1.53	0.90
3:G:132:TRP:HE1	3:G:143:THR:HB	1.35	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:113:VAL:HB	3:K:160:MET:HE1	1.53	0.90
1:A:62:SER:HB3	1:A:73:VAL:H	1.35	0.90
1:A:361:THR:HG22	1:A:362:ASP:H	1.36	0.89
1:E:366:LEU:HD12	1:E:370:GLU:OE2	1.71	0.89
2:F:138:ILE:C	2:F:140:MET:H	1.80	0.89
1:I:105:LEU:HD23	1:I:137:ALA:HA	1.54	0.89
1:A:338:LEU:O	1:A:340:PRO:HD3	1.72	0.89
1:E:269:ILE:HB	1:E:270:PRO:HD2	1.54	0.89
3:G:138:ARG:NH2	3:G:138:ARG:HB3	1.86	0.89
1:A:329:GLU:HG2	1:A:330:TYR:H	1.34	0.89
3:C:90:ARG:HB2	3:C:90:ARG:NH2	1.87	0.89
1:E:157:ILE:H	1:E:157:ILE:HD12	1.35	0.89
2:F:142:LEU:H	2:F:142:LEU:HD12	1.35	0.89
2:J:82:ALA:HB2	2:J:231:MET:HE2	1.53	0.89
2:F:131:VAL:HB	2:F:132:PRO:HD3	1.55	0.89
3:G:22:ARG:HH12	3:G:25:TRP:HA	1.36	0.89
2:J:71:ILE:O	2:J:74:VAL:HG22	1.72	0.89
3:K:138:ARG:NH2	3:K:138:ARG:HB3	1.86	0.89
3:C:77:GLY:HA2	3:C:159:ILE:HG23	1.55	0.89
1:I:361:THR:HG22	1:I:362:ASP:H	1.36	0.89
3:K:90:ARG:HB2	3:K:90:ARG:NH2	1.87	0.89
1:A:66:LEU:CD1	1:A:72:MET:HB2	2.03	0.89
1:A:107:ARG:HB3	2:B:192:HIS:HA	1.54	0.89
1:E:66:LEU:CD1	1:E:72:MET:HB2	2.03	0.89
1:E:282:ILE:C	1:E:283:ILE:HG12	1.98	0.89
1:I:366:LEU:HD12	1:I:370:GLU:OE2	1.71	0.88
2:J:142:LEU:H	2:J:142:LEU:HD12	1.35	0.88
1:E:338:LEU:O	1:E:340:PRO:HD3	1.72	0.88
2:B:98:VAL:HG21	2:B:133:ALA:HB2	1.56	0.88
2:B:131:VAL:HB	2:B:132:PRO:HD3	1.55	0.88
2:F:71:ILE:O	2:F:74:VAL:HG22	1.72	0.88
1:I:107:ARG:HB3	2:J:192:HIS:HA	1.54	0.88
3:G:77:GLY:HA2	3:G:159:ILE:HG23	1.55	0.88
2:J:201:TYR:HD1	2:J:203:ARG:HD2	1.38	0.88
2:F:128:ALA:H	2:F:165:ASN:HD21	1.20	0.88
1:E:361:THR:HG22	1:E:362:ASP:H	1.36	0.88
2:F:98:VAL:HG21	2:F:133:ALA:HB2	1.55	0.88
2:B:201:TYR:HD1	2:B:203:ARG:HD2	1.38	0.87
2:B:240:GLY:O	2:B:244:SER:N	2.06	0.87
2:B:71:ILE:O	2:B:74:VAL:HG22	1.72	0.87
2:B:128:ALA:H	2:B:165:ASN:HD21	1.20	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:22:ARG:HH12	3:K:25:TRP:HA	1.36	0.87
1:E:107:ARG:HB3	2:F:192:HIS:HA	1.54	0.87
2:F:243:TYR:C	2:F:245:THR:H	1.82	0.87
2:J:26:THR:O	2:J:30:PHE:HB2	1.75	0.87
2:J:243:TYR:C	2:J:245:THR:H	1.82	0.87
1:E:52:ARG:NH1	1:E:398:GLN:HB3	1.90	0.87
2:F:240:GLY:O	2:F:244:SER:N	2.06	0.87
1:I:66:LEU:CD1	1:I:72:MET:HB2	2.03	0.87
2:J:240:GLY:O	2:J:244:SER:N	2.06	0.87
2:F:201:TYR:HD1	2:F:203:ARG:HD2	1.38	0.87
3:K:77:GLY:HA2	3:K:159:ILE:HG23	1.55	0.87
2:B:138:ILE:C	2:B:140:MET:H	1.80	0.86
1:E:187:LEU:HD11	2:F:189:VAL:HG22	1.56	0.86
2:F:26:THR:O	2:F:30:PHE:HB2	1.75	0.86
2:B:26:THR:O	2:B:30:PHE:HB2	1.75	0.86
1:A:282:ILE:C	1:A:283:ILE:HG12	1.98	0.86
2:F:229:SER:C	2:F:231:MET:H	1.78	0.86
2:F:244:SER:HA	2:F:247:LYS:HZ2	1.40	0.86
1:I:269:ILE:HB	1:I:270:PRO:HD2	1.54	0.86
1:I:282:ILE:C	1:I:283:ILE:HG12	1.98	0.86
2:J:98:VAL:HG21	2:J:133:ALA:HB2	1.56	0.86
1:I:187:LEU:HD11	2:J:189:VAL:HG22	1.56	0.86
2:J:138:ILE:C	2:J:140:MET:H	1.80	0.86
1:A:187:LEU:HD11	2:B:189:VAL:HG22	1.56	0.86
1:I:203:MET:HE3	2:J:102:LEU:HB3	1.58	0.86
1:A:52:ARG:NH1	1:A:398:GLN:HB3	1.90	0.86
1:E:203:MET:HE3	2:F:102:LEU:HB3	1.58	0.86
2:J:131:VAL:HB	2:J:132:PRO:HD3	1.55	0.86
1:E:72:MET:HB3	1:E:135:LEU:HD11	1.58	0.86
2:F:211:ARG:HH22	3:G:158:SER:HA	1.38	0.86
1:I:52:ARG:NH1	1:I:398:GLN:HB3	1.90	0.86
1:I:315:VAL:O	1:I:374:ILE:HG23	1.76	0.86
2:J:211:ARG:HH22	3:K:158:SER:HA	1.38	0.86
1:I:200:PHE:HB3	1:I:201:PRO:HD3	1.57	0.86
2:J:128:ALA:H	2:J:165:ASN:HD21	1.20	0.85
1:A:200:PHE:HB3	1:A:201:PRO:HD3	1.57	0.85
1:E:307:PRO:HG2	1:E:308:GLY:H	1.42	0.85
1:A:72:MET:HB3	1:A:135:LEU:HD11	1.58	0.85
3:G:41:TYR:HE2	5:N:3:UNK:HA	1.41	0.85
1:I:307:PRO:HG2	1:I:308:GLY:H	1.42	0.85
1:E:200:PHE:HB3	1:E:201:PRO:HD3	1.57	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:68:THR:HG21	5:O:7:UNK:CB	2.07	0.85
3:K:69:GLU:HB2	3:K:152:MET:HE3	1.58	0.85
2:B:243:TYR:C	2:B:245:THR:H	1.82	0.84
1:I:63:LYS:H	1:I:72:MET:HG3	1.41	0.84
1:I:210:ILE:HA	2:J:92:PHE:CE1	2.12	0.84
1:A:315:VAL:O	1:A:374:ILE:HG23	1.76	0.84
1:E:63:LYS:H	1:E:72:MET:HG3	1.41	0.84
1:E:315:VAL:O	1:E:374:ILE:HG23	1.76	0.84
2:B:239:VAL:HG12	2:J:205:VAL:HG22	1.56	0.84
2:F:238:PHE:HB2	2:F:241:LYS:CD	2.08	0.84
1:A:210:ILE:HA	2:B:92:PHE:CE1	2.12	0.84
1:A:63:LYS:H	1:A:72:MET:HG3	1.41	0.84
3:G:69:GLU:HB2	3:G:152:MET:HE3	1.59	0.84
1:A:307:PRO:HG2	1:A:308:GLY:H	1.42	0.84
3:G:68:THR:HG21	5:N:7:UNK:CB	2.07	0.84
3:C:69:GLU:HB2	3:C:152:MET:HE3	1.58	0.84
3:G:44:ILE:HG22	3:G:45:TYR:N	1.93	0.84
1:A:305:LYS:HG3	1:A:310:GLU:H	1.43	0.84
2:B:143:SER:HB3	2:B:148:ILE:HD12	1.60	0.84
1:E:359:LEU:HD21	1:E:376:VAL:CG1	2.05	0.84
1:E:210:ILE:HA	2:F:92:PHE:CE1	2.12	0.84
1:A:202:TRP:C	1:A:204:ILE:H	1.85	0.84
3:C:44:ILE:HG22	3:C:45:TYR:N	1.93	0.84
1:E:309:ARG:CD	1:E:381:ALA:HA	2.08	0.84
3:K:44:ILE:HG22	3:K:45:TYR:N	1.93	0.84
2:B:201:TYR:CD1	2:B:203:ARG:HD2	2.13	0.83
1:I:298:GLU:OE2	1:I:316:LYS:HB2	1.78	0.83
2:F:82:ALA:HB1	2:F:146:TYR:OH	1.78	0.83
4:H:505:UNK:C	4:H:507:UNK:N	2.38	0.83
2:J:199:PRO:HG2	3:K:138:ARG:HG3	1.60	0.83
1:A:359:LEU:HD21	1:A:376:VAL:CG1	2.06	0.83
1:E:298:GLU:OE2	1:E:316:LYS:HB2	1.78	0.83
2:F:143:SER:HB3	2:F:148:ILE:HD12	1.60	0.83
2:J:238:PHE:HB2	2:J:241:LYS:CD	2.08	0.83
2:B:82:ALA:HB1	2:B:146:TYR:OH	1.78	0.83
2:B:238:PHE:HB2	2:B:241:LYS:CD	2.08	0.83
1:I:309:ARG:CD	1:I:381:ALA:HA	2.07	0.83
1:A:203:MET:HE3	2:B:102:LEU:HB3	1.58	0.83
1:A:305:LYS:HE2	1:A:310:GLU:HB2	1.60	0.83
1:E:213:TRP:NE1	2:F:91:PRO:HG2	1.93	0.83
2:J:201:TYR:CD1	2:J:203:ARG:HD2	2.13	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:211:ARG:HH22	3:C:158:SER:HA	1.38	0.83
3:C:41:TYR:HE2	5:M:3:UNK:HA	1.41	0.83
3:C:68:THR:HG21	5:M:7:UNK:CB	2.07	0.83
1:E:305:LYS:HE2	1:E:310:GLU:HB2	1.60	0.83
1:I:72:MET:HB3	1:I:135:LEU:HD11	1.58	0.83
3:K:96:ALA:HB3	3:K:99:GLU:HB2	1.60	0.83
1:E:305:LYS:HG3	1:E:310:GLU:H	1.43	0.83
1:I:299:LEU:HD11	1:I:417:ILE:HB	1.60	0.83
1:A:139:ARG:HD2	2:B:118:TYR:CE1	2.13	0.83
1:E:139:ARG:HD2	2:F:118:TYR:CE1	2.13	0.83
3:G:96:ALA:HB3	3:G:99:GLU:HB2	1.61	0.83
1:I:399:ILE:HG12	1:I:400:GLY:H	1.44	0.83
3:K:148:ILE:HA	3:K:152:MET:HB2	1.60	0.83
1:A:399:ILE:HG12	1:A:400:GLY:H	1.44	0.83
2:F:201:TYR:CD1	2:F:203:ARG:HD2	2.13	0.83
4:L:505:UNK:C	4:L:507:UNK:N	2.38	0.83
1:A:105:LEU:HD22	1:A:135:LEU:HD13	1.60	0.82
2:F:245:THR:HG22	2:F:246:THR:N	1.94	0.82
3:K:81:ALA:HA	3:K:166:PHE:HE2	1.42	0.82
2:B:199:PRO:HG2	3:C:138:ARG:HG3	1.60	0.82
1:E:261:THR:HG21	2:F:167:PRO:CA	2.08	0.82
1:I:105:LEU:HD22	1:I:135:LEU:HD13	1.60	0.82
1:I:305:LYS:HG3	1:I:310:GLU:H	1.43	0.82
3:K:41:TYR:HE2	5:O:3:UNK:HA	1.41	0.82
1:E:202:TRP:C	1:E:204:ILE:H	1.85	0.82
1:E:399:ILE:HG12	1:E:400:GLY:H	1.44	0.82
3:G:148:ILE:HA	3:G:152:MET:HB2	1.60	0.82
2:J:143:SER:HB3	2:J:148:ILE:HD12	1.60	0.82
2:J:145:SER:H	2:J:148:ILE:HD11	1.44	0.82
3:C:45:TYR:CD1	3:C:61:TYR:HB3	2.15	0.82
1:I:329:GLU:HB3	1:I:404:MET:HB2	1.61	0.82
2:J:82:ALA:HB1	2:J:146:TYR:OH	1.78	0.82
1:E:299:LEU:HD11	1:E:417:ILE:HB	1.61	0.82
3:K:45:TYR:CD1	3:K:61:TYR:HB3	2.15	0.82
3:K:81:ALA:HA	3:K:166:PHE:CE2	2.15	0.82
1:A:298:GLU:OE2	1:A:316:LYS:HB2	1.78	0.82
1:A:299:LEU:HD11	1:A:417:ILE:HB	1.61	0.82
3:C:81:ALA:HA	3:C:166:PHE:CE2	2.15	0.82
3:C:96:ALA:HB3	3:C:99:GLU:HB2	1.61	0.82
1:A:213:TRP:NE1	2:B:91:PRO:HG2	1.93	0.82
1:A:263:SER:C	1:A:265:PHE:H	1.87	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:383:TRP:CD1	1:E:388:LEU:HD12	2.14	0.82
1:I:139:ARG:HD2	2:J:118:TYR:CE1	2.13	0.82
1:I:213:TRP:NE1	2:J:91:PRO:HG2	1.93	0.82
2:B:145:SER:H	2:B:148:ILE:HD11	1.44	0.82
2:F:219:PRO:O	2:F:220:VAL:HG23	1.80	0.82
1:I:305:LYS:HE2	1:I:310:GLU:HB2	1.60	0.82
2:F:199:PRO:HG2	3:G:138:ARG:HG3	1.60	0.81
1:I:359:LEU:HD21	1:I:376:VAL:CG1	2.05	0.81
3:C:81:ALA:HA	3:C:166:PHE:HE2	1.42	0.81
3:C:148:ILE:HA	3:C:152:MET:HB2	1.60	0.81
1:E:305:LYS:O	1:E:306:VAL:HG23	1.81	0.81
1:I:383:TRP:CD1	1:I:388:LEU:HD12	2.14	0.81
1:A:119:ARG:CD	1:A:273:ALA:HA	2.10	0.81
1:A:383:TRP:CD1	1:A:388:LEU:HD12	2.14	0.81
2:B:177:GLU:HG3	1:I:422:ILE:HG12	1.60	0.81
1:E:216:LYS:HE2	1:E:239:ASP:OD1	1.81	0.81
1:E:329:GLU:HB3	1:E:404:MET:HB2	1.61	0.81
1:I:261:THR:HG21	2:J:167:PRO:CA	2.08	0.81
1:A:119:ARG:HG2	1:A:274:GLY:H	1.44	0.81
2:F:120:PRO:HD2	2:F:123:LEU:HD22	1.63	0.81
1:E:119:ARG:CD	1:E:273:ALA:HA	2.11	0.81
2:F:205:VAL:HG13	2:J:239:VAL:O	1.79	0.81
3:G:81:ALA:HA	3:G:166:PHE:CE2	2.15	0.81
3:G:81:ALA:HA	3:G:166:PHE:HE2	1.42	0.81
2:J:219:PRO:O	2:J:220:VAL:HG23	1.80	0.81
1:A:309:ARG:CD	1:A:381:ALA:HA	2.08	0.81
2:B:219:PRO:O	2:B:220:VAL:HG23	1.80	0.81
3:G:45:TYR:CD1	3:G:61:TYR:HB3	2.15	0.81
1:I:263:SER:C	1:I:265:PHE:H	1.87	0.81
1:A:216:LYS:HE2	1:A:239:ASP:OD1	1.81	0.81
1:E:119:ARG:HG2	1:E:274:GLY:H	1.44	0.81
1:I:119:ARG:HG2	1:I:274:GLY:H	1.44	0.81
1:I:202:TRP:C	1:I:204:ILE:H	1.85	0.81
2:F:145:SER:H	2:F:148:ILE:HD11	1.44	0.80
1:A:261:THR:HG21	2:B:167:PRO:CA	2.08	0.80
1:A:329:GLU:HB3	1:A:404:MET:HB2	1.61	0.80
1:E:105:LEU:HD22	1:E:135:LEU:HD13	1.60	0.80
2:J:121:ILE:H	2:J:121:ILE:CD1	1.95	0.80
2:J:120:PRO:HD2	2:J:123:LEU:HD22	1.63	0.80
1:I:216:LYS:HE2	1:I:239:ASP:OD1	1.81	0.80
3:C:143:THR:HB	3:C:144:PRO:HD2	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:119:ARG:CD	1:I:273:ALA:HA	2.10	0.80
1:I:261:THR:CG2	2:J:167:PRO:HA	2.12	0.80
2:B:74:VAL:O	2:B:76:PHE:N	2.15	0.80
1:A:305:LYS:O	1:A:306:VAL:HG23	1.81	0.80
1:I:305:LYS:O	1:I:306:VAL:HG23	1.81	0.80
2:B:245:THR:HG22	2:B:246:THR:N	1.94	0.80
1:E:105:LEU:HD13	1:E:135:LEU:HD22	1.64	0.80
1:E:207:ALA:HA	1:E:210:ILE:HD12	1.64	0.80
2:J:245:THR:HG22	2:J:246:THR:N	1.94	0.80
2:B:120:PRO:HD2	2:B:123:LEU:HD22	1.63	0.80
1:E:261:THR:CG2	2:F:167:PRO:HA	2.12	0.80
1:E:263:SER:C	1:E:265:PHE:H	1.87	0.80
1:I:258:TYR:O	1:I:262:ASN:HB2	1.82	0.80
1:E:107:ARG:HH21	2:F:191:PHE:HD1	1.30	0.79
1:A:107:ARG:HH21	2:B:191:PHE:HD1	1.30	0.79
1:I:207:ALA:HA	1:I:210:ILE:HD12	1.64	0.79
2:J:74:VAL:O	2:J:76:PHE:N	2.15	0.79
1:E:56:TRP:CD2	1:E:159:GLY:HA3	2.18	0.79
1:I:56:TRP:CD2	1:I:159:GLY:HA3	2.18	0.79
1:I:196:TYR:H	1:I:196:TYR:HD2	1.29	0.79
1:A:258:TYR:O	1:A:262:ASN:HB2	1.82	0.79
3:G:89:ASP:OD1	3:G:92:VAL:HA	1.82	0.79
1:I:306:VAL:HG11	1:I:425:PHE:HD1	1.48	0.79
1:A:261:THR:CG2	2:B:167:PRO:HA	2.11	0.79
2:F:205:VAL:HG22	2:J:239:VAL:HG12	1.65	0.79
3:K:143:THR:HB	3:K:144:PRO:HD2	1.63	0.79
1:I:59:VAL:HA	1:I:75:SER:O	1.84	0.78
1:A:104:VAL:HG21	1:A:143:TRP:NE1	1.97	0.78
1:I:105:LEU:HD13	1:I:135:LEU:HD22	1.64	0.78
2:J:79:ALA:HA	2:J:231:MET:HG3	1.66	0.78
1:A:56:TRP:CD2	1:A:159:GLY:HA3	2.18	0.78
1:A:196:TYR:H	1:A:196:TYR:HD2	1.29	0.78
1:A:207:ALA:HA	1:A:210:ILE:HD12	1.64	0.78
4:D:505:UNK:C	4:D:507:UNK:N	2.38	0.78
3:K:41:TYR:CE2	5:O:3:UNK:HA	2.19	0.78
2:F:74:VAL:O	2:F:76:PHE:N	2.15	0.78
2:F:79:ALA:HA	2:F:231:MET:HG3	1.66	0.78
2:F:134:LEU:C	2:F:136:LEU:H	1.92	0.78
3:K:132:TRP:HE1	3:K:144:PRO:HD2	1.47	0.78
1:A:266:PRO:CD	1:A:267:ARG:H	1.97	0.78
1:I:266:PRO:CD	1:I:267:ARG:H	1.97	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:235:LEU:HD23	2:J:235:LEU:C	2.09	0.78
2:J:238:PHE:O	2:J:240:GLY:N	2.17	0.78
3:C:67:TRP:O	3:C:71:PRO:HG2	1.84	0.78
2:F:235:LEU:HD23	2:F:235:LEU:C	2.09	0.78
2:B:128:ALA:H	2:B:165:ASN:ND2	1.81	0.78
2:B:235:LEU:HD23	2:B:235:LEU:C	2.09	0.78
3:C:89:ASP:OD1	3:C:92:VAL:HA	1.83	0.78
1:E:306:VAL:HG11	1:E:425:PHE:HD1	1.48	0.78
3:G:41:TYR:CE2	5:N:3:UNK:HA	2.19	0.78
3:G:132:TRP:HE1	3:G:144:PRO:HD2	1.47	0.78
3:G:143:THR:HB	3:G:144:PRO:HD2	1.63	0.78
2:J:65:TRP:O	2:J:67:THR:N	2.17	0.78
3:K:89:ASP:OD1	3:K:92:VAL:HA	1.83	0.78
1:E:258:TYR:O	1:E:262:ASN:HB2	1.82	0.78
1:E:266:PRO:CD	1:E:267:ARG:H	1.97	0.78
1:I:104:VAL:HG21	1:I:143:TRP:NE1	1.97	0.78
2:J:246:THR:C	2:J:247:LYS:HD2	2.09	0.77
2:B:134:LEU:C	2:B:136:LEU:H	1.92	0.77
2:B:238:PHE:O	2:B:240:GLY:N	2.17	0.77
1:E:59:VAL:HA	1:E:75:SER:O	1.84	0.77
1:E:178:THR:OG1	1:E:184:THR:HA	1.84	0.77
1:A:59:VAL:HA	1:A:75:SER:O	1.84	0.77
1:A:201:PRO:HA	1:A:204:ILE:CD1	2.15	0.77
2:B:102:LEU:O	2:B:106:TRP:HB2	1.84	0.77
1:E:51:MET:SD	1:E:399:ILE:HG13	2.24	0.77
1:E:110:GLN:O	1:E:116:PHE:HB2	1.85	0.77
2:F:128:ALA:H	2:F:165:ASN:ND2	1.81	0.77
2:F:160:LEU:O	2:F:163:PRO:HG2	1.85	0.77
2:F:246:THR:C	2:F:247:LYS:HD2	2.09	0.77
2:J:128:ALA:H	2:J:165:ASN:ND2	1.81	0.77
2:J:160:LEU:O	2:J:163:PRO:HG2	1.85	0.77
1:A:51:MET:SD	1:A:399:ILE:HG13	2.25	0.77
1:A:84:TRP:CE2	1:A:91:PRO:HD3	2.20	0.77
2:B:65:TRP:O	2:B:67:THR:N	2.17	0.77
2:B:121:ILE:H	2:B:121:ILE:CD1	1.95	0.77
3:C:19:VAL:HA	3:C:102:ARG:HD3	1.66	0.77
3:C:108:VAL:O	3:C:108:VAL:HG12	1.85	0.77
1:E:84:TRP:CE2	1:E:91:PRO:HD3	2.20	0.77
1:A:105:LEU:HD13	1:A:135:LEU:HD22	1.64	0.77
1:I:201:PRO:HA	1:I:204:ILE:CD1	2.15	0.77
3:C:41:TYR:CE2	5:M:3:UNK:HA	2.19	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:178:THR:OG1	1:I:184:THR:HA	1.84	0.77
2:B:246:THR:C	2:B:247:LYS:HD2	2.09	0.77
1:A:306:VAL:HG11	1:A:425:PHE:HD1	1.48	0.77
3:C:132:TRP:HE1	3:C:144:PRO:HD2	1.47	0.77
3:G:19:VAL:HA	3:G:102:ARG:HD3	1.66	0.77
2:F:238:PHE:O	2:F:240:GLY:N	2.17	0.77
2:J:102:LEU:O	2:J:106:TRP:HB2	1.84	0.77
3:K:108:VAL:O	3:K:108:VAL:HG12	1.85	0.77
2:B:13:PHE:CG	2:B:19:ALA:HA	2.19	0.76
1:E:196:TYR:H	1:E:196:TYR:HD2	1.29	0.76
2:J:13:PHE:CG	2:J:19:ALA:HA	2.19	0.76
3:K:67:TRP:O	3:K:71:PRO:HG2	1.84	0.76
3:G:128:GLN:O	3:G:131:THR:HG22	1.85	0.76
2:J:134:LEU:C	2:J:136:LEU:H	1.92	0.76
3:C:128:GLN:O	3:C:131:THR:HG22	1.85	0.76
1:E:201:PRO:HA	1:E:204:ILE:CD1	2.15	0.76
3:G:154:TYR:HB2	3:G:155:PRO:HD3	1.67	0.76
1:I:51:MET:SD	1:I:399:ILE:HG13	2.25	0.76
1:I:84:TRP:CE2	1:I:91:PRO:HD3	2.19	0.76
1:A:178:THR:OG1	1:A:184:THR:HA	1.84	0.76
3:C:22:ARG:NH1	3:C:22:ARG:HB3	2.01	0.76
2:F:13:PHE:CG	2:F:19:ALA:HA	2.19	0.76
2:F:102:LEU:O	2:F:106:TRP:HB2	1.84	0.76
3:G:138:ARG:HB3	3:G:138:ARG:HH21	1.50	0.76
1:A:110:GLN:O	1:A:116:PHE:HB2	1.85	0.76
2:B:160:LEU:O	2:B:163:PRO:HG2	1.85	0.76
2:F:83:PHE:HE2	4:H:507:UNK:CB	1.99	0.76
3:K:80:LEU:O	3:K:84:LEU:HB2	1.86	0.76
2:B:243:TYR:O	2:B:245:THR:N	2.17	0.76
2:J:243:TYR:O	2:J:245:THR:N	2.17	0.76
3:K:154:TYR:HB2	3:K:155:PRO:HD3	1.67	0.76
2:B:79:ALA:HA	2:B:231:MET:HG3	1.66	0.76
3:G:67:TRP:O	3:G:71:PRO:HG2	1.84	0.76
3:G:80:LEU:O	3:G:84:LEU:HB2	1.86	0.76
2:J:65:TRP:HB3	2:J:66:PRO:HD3	1.68	0.76
1:E:104:VAL:HG21	1:E:143:TRP:NE1	1.97	0.76
3:G:22:ARG:HB3	3:G:22:ARG:NH1	2.01	0.76
2:B:65:TRP:HB3	2:B:66:PRO:HD3	1.68	0.76
1:I:110:GLN:O	1:I:116:PHE:HB2	1.85	0.76
2:B:57:VAL:HG23	2:B:123:LEU:O	1.86	0.75
2:B:83:PHE:HE2	4:D:507:UNK:CB	1.99	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:96:LEU:HD13	1:E:112:ILE:HB	1.68	0.75
1:E:202:TRP:C	1:E:204:ILE:N	2.44	0.75
2:F:243:TYR:O	2:F:245:THR:N	2.17	0.75
3:K:22:ARG:NH1	3:K:22:ARG:HB3	2.01	0.75
2:F:57:VAL:HG23	2:F:123:LEU:O	1.87	0.75
3:G:108:VAL:O	3:G:108:VAL:HG12	1.85	0.75
1:I:237:ASP:HA	1:I:240:ARG:HG2	1.68	0.75
2:J:151:VAL:HA	2:J:237:TRP:CE2	2.22	0.75
2:F:164:ASN:O	2:F:167:PRO:HD2	1.86	0.75
3:C:31:LEU:HD11	3:C:35:TYR:HD1	1.51	0.75
3:C:69:GLU:CD	3:C:152:MET:HG2	2.12	0.75
1:E:237:ASP:HA	1:E:240:ARG:HG2	1.67	0.75
3:G:31:LEU:HD11	3:G:35:TYR:HD1	1.51	0.75
2:J:57:VAL:HG23	2:J:123:LEU:O	1.86	0.75
3:K:19:VAL:HA	3:K:102:ARG:HD3	1.66	0.75
1:A:96:LEU:HD13	1:A:112:ILE:HB	1.68	0.75
2:J:83:PHE:HE2	4:L:507:UNK:CB	1.99	0.75
2:F:119:PHE:HB3	2:F:123:LEU:HD21	1.69	0.75
3:G:69:GLU:CD	3:G:152:MET:HG2	2.12	0.75
2:J:164:ASN:O	2:J:167:PRO:HD2	1.87	0.75
3:K:62:TRP:CZ2	3:K:144:PRO:HB3	2.22	0.75
3:K:69:GLU:CD	3:K:152:MET:HG2	2.12	0.75
3:K:128:GLN:O	3:K:131:THR:HG22	1.85	0.75
1:A:99:GLY:O	1:A:101:PRO:HD3	1.87	0.75
1:A:237:ASP:HA	1:A:240:ARG:HG2	1.67	0.75
2:B:138:ILE:C	2:B:140:MET:N	2.42	0.75
2:F:185:LEU:O	2:F:189:VAL:HG23	1.87	0.75
3:G:69:GLU:CB	3:G:152:MET:HE3	2.17	0.75
1:I:96:LEU:HD13	1:I:112:ILE:HB	1.69	0.75
2:B:185:LEU:O	2:B:189:VAL:HG23	1.87	0.75
2:B:239:VAL:HG12	2:J:205:VAL:CG2	2.17	0.75
3:C:62:TRP:CZ2	3:C:144:PRO:HB3	2.22	0.75
3:K:159:ILE:O	3:K:162:VAL:HG22	1.87	0.75
1:A:202:TRP:C	1:A:204:ILE:N	2.44	0.74
2:B:216:GLU:OE2	2:B:216:GLU:HA	1.86	0.74
1:E:277:LYS:N	1:E:278:PRO:HD2	2.02	0.74
2:F:65:TRP:HB3	2:F:66:PRO:HD3	1.68	0.74
2:J:119:PHE:HB3	2:J:123:LEU:HD21	1.69	0.74
2:B:119:PHE:HB3	2:B:123:LEU:HD21	1.69	0.74
2:B:151:VAL:HA	2:B:237:TRP:CE2	2.22	0.74
3:C:138:ARG:HB3	3:C:138:ARG:HH21	1.50	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:224:LEU:HD11	4:L:519:UNK:HA	1.69	0.74
1:A:277:LYS:N	1:A:278:PRO:HD2	2.02	0.74
2:F:176:THR:HG21	2:F:178:GLN:HE22	1.53	0.74
2:F:205:VAL:CG2	2:J:239:VAL:HG12	2.18	0.74
2:F:245:THR:O	2:F:247:LYS:N	2.17	0.74
1:I:99:GLY:O	1:I:101:PRO:HD3	1.87	0.74
1:I:107:ARG:HH21	2:J:191:PHE:HD1	1.30	0.74
1:A:67:ASN:O	1:A:69:ASN:N	2.20	0.74
3:C:80:LEU:O	3:C:84:LEU:HB2	1.86	0.74
1:E:224:LEU:HD11	4:H:519:UNK:HA	1.69	0.74
2:F:151:VAL:HA	2:F:237:TRP:CE2	2.22	0.74
1:I:277:LYS:N	1:I:278:PRO:HD2	2.02	0.74
2:J:185:LEU:O	2:J:189:VAL:HG23	1.87	0.74
2:B:164:ASN:O	2:B:167:PRO:HD2	1.86	0.74
1:I:250:THR:HG21	2:J:134:LEU:HD12	1.70	0.74
2:J:108:ASN:ND2	3:K:127:GLU:HB3	2.03	0.74
3:C:80:LEU:H	3:C:80:LEU:HD22	1.53	0.74
3:C:154:TYR:HB2	3:C:155:PRO:HD3	1.67	0.74
3:C:159:ILE:O	3:C:162:VAL:HG22	1.87	0.74
1:E:99:GLY:O	1:E:101:PRO:HD3	1.87	0.74
1:I:196:TYR:HH	2:J:110:TYR:HE1	1.35	0.74
2:F:49:THR:HB	2:F:72:LEU:HD13	1.70	0.74
2:F:108:ASN:ND2	3:G:127:GLU:HB3	2.03	0.74
2:F:121:ILE:H	2:F:121:ILE:CD1	1.95	0.74
2:F:216:GLU:HA	2:F:216:GLU:OE2	1.86	0.74
1:I:89:ALA:HB3	1:I:153:GLY:O	1.88	0.74
1:A:42:GLU:H	1:A:158:ILE:HD11	1.52	0.74
2:B:33:LEU:HD23	2:B:33:LEU:C	2.13	0.74
3:G:22:ARG:HH12	3:G:25:TRP:CA	2.01	0.74
1:I:202:TRP:C	1:I:204:ILE:N	2.44	0.74
2:J:49:THR:HB	2:J:72:LEU:HD13	1.70	0.74
3:K:80:LEU:H	3:K:80:LEU:HD22	1.53	0.74
1:A:89:ALA:HB3	1:A:153:GLY:O	1.88	0.73
3:C:69:GLU:CB	3:C:152:MET:HE3	2.17	0.73
3:K:31:LEU:HD11	3:K:35:TYR:HD1	1.51	0.73
1:A:250:THR:HG21	2:B:134:LEU:HD12	1.70	0.73
1:I:42:GLU:H	1:I:158:ILE:HD11	1.52	0.73
1:A:306:VAL:HG11	1:A:425:PHE:CD1	2.23	0.73
3:C:22:ARG:HH12	3:C:25:TRP:CA	2.01	0.73
1:E:42:GLU:H	1:E:158:ILE:HD11	1.52	0.73
3:G:159:ILE:O	3:G:162:VAL:HG22	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:306:VAL:HG11	1:I:425:PHE:CD1	2.23	0.73
3:K:69:GLU:CB	3:K:152:MET:HE3	2.17	0.73
1:E:306:VAL:HG11	1:E:425:PHE:CD1	2.23	0.73
2:F:120:PRO:C	2:F:122:SER:H	1.96	0.73
1:E:66:LEU:HD13	1:E:70:GLU:O	1.89	0.73
2:F:65:TRP:O	2:F:67:THR:N	2.17	0.73
2:F:138:ILE:C	2:F:140:MET:N	2.42	0.73
2:J:175:ALA:HB1	2:J:182:LEU:HD11	1.70	0.73
2:B:108:ASN:ND2	3:C:127:GLU:HB3	2.03	0.73
2:J:33:LEU:HD23	2:J:33:LEU:C	2.13	0.73
3:K:138:ARG:HB3	3:K:138:ARG:HH21	1.50	0.73
3:G:62:TRP:CZ2	3:G:144:PRO:HB3	2.22	0.73
3:G:80:LEU:HD22	3:G:80:LEU:H	1.53	0.73
3:G:107:LEU:O	3:G:111:LEU:HD12	1.89	0.73
2:F:175:ALA:HB1	2:F:182:LEU:HD11	1.70	0.73
1:I:67:ASN:O	1:I:69:ASN:N	2.21	0.73
1:E:89:ALA:HB3	1:E:153:GLY:O	1.88	0.73
2:F:33:LEU:HD23	2:F:33:LEU:C	2.13	0.73
1:I:388:LEU:C	1:I:390:ASP:H	1.97	0.73
3:C:107:LEU:O	3:C:111:LEU:HD12	1.89	0.73
1:E:67:ASN:O	1:E:69:ASN:N	2.20	0.73
1:E:123:LEU:HD12	1:E:123:LEU:N	2.04	0.73
2:J:176:THR:HG21	2:J:178:GLN:HE22	1.53	0.73
3:K:22:ARG:HH12	3:K:25:TRP:CA	2.01	0.73
3:K:107:LEU:O	3:K:111:LEU:HD12	1.89	0.73
1:A:80:VAL:HG23	1:A:127:LYS:O	1.89	0.72
1:A:224:LEU:HD11	4:D:519:UNK:HA	1.69	0.72
3:C:169:LYS:HZ3	3:C:176:ALA:HA	1.53	0.72
1:I:213:TRP:HE1	2:J:91:PRO:CG	1.98	0.72
1:A:399:ILE:HG12	1:A:400:GLY:N	2.04	0.72
2:B:91:PRO:HG3	2:B:141:LEU:HG	1.71	0.72
2:B:176:THR:HG21	2:B:178:GLN:HE22	1.53	0.72
1:E:104:VAL:HG11	1:E:143:TRP:CE2	2.24	0.72
2:J:75:THR:HG23	2:J:75:THR:O	1.90	0.72
1:A:213:TRP:HE1	2:B:91:PRO:CG	1.98	0.72
3:G:111:LEU:HD22	4:H:510:UNK:CB	2.20	0.72
1:A:123:LEU:N	1:A:123:LEU:HD12	2.04	0.72
2:B:44:ILE:HG12	3:C:126:THR:HG21	1.71	0.72
2:B:120:PRO:C	2:B:122:SER:H	1.96	0.72
2:B:199:PRO:CG	3:C:138:ARG:HG3	2.20	0.72
1:I:63:LYS:HG3	1:I:65:SER:H	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:104:VAL:HG11	1:I:143:TRP:CE2	2.24	0.72
1:I:123:LEU:HD12	1:I:123:LEU:N	2.04	0.72
2:J:216:GLU:OE2	2:J:216:GLU:HA	1.87	0.72
1:A:63:LYS:HG3	1:A:65:SER:H	1.54	0.72
2:B:175:ALA:HB1	2:B:182:LEU:HD11	1.70	0.72
2:B:245:THR:O	2:B:247:LYS:N	2.17	0.72
1:E:213:TRP:HE1	2:F:91:PRO:CG	1.98	0.72
1:E:222:SER:CA	1:E:225:ARG:HB3	2.19	0.72
2:F:199:PRO:CG	3:G:138:ARG:HG3	2.20	0.72
2:J:13:PHE:HB3	2:J:19:ALA:HB2	1.71	0.72
2:J:138:ILE:C	2:J:140:MET:N	2.42	0.72
1:A:66:LEU:HD13	1:A:70:GLU:O	1.89	0.72
1:A:104:VAL:HG11	1:A:143:TRP:CE2	2.24	0.72
2:B:47:MET:HE1	3:C:126:THR:O	1.90	0.72
2:B:203:ARG:HB3	2:B:207:ARG:NH2	2.05	0.72
2:B:210:LEU:C	2:B:212:THR:N	2.45	0.72
2:B:228:VAL:C	2:B:230:MET:H	1.97	0.72
1:E:144:HIS:HD1	1:E:163:TRP:CD1	2.07	0.72
1:E:329:GLU:HG2	1:E:330:TYR:N	2.05	0.72
2:F:123:LEU:HG	2:F:124:VAL:HG13	1.72	0.72
1:I:222:SER:CA	1:I:225:ARG:HB3	2.19	0.72
2:B:66:PRO:C	2:B:70:PRO:HG2	2.15	0.72
1:I:329:GLU:HG2	1:I:330:TYR:N	2.05	0.72
1:I:399:ILE:HG12	1:I:400:GLY:N	2.04	0.72
2:B:49:THR:HB	2:B:72:LEU:HD13	1.70	0.72
2:B:55:PHE:O	2:B:124:VAL:HA	1.90	0.72
2:F:44:ILE:HG12	3:G:126:THR:HG21	1.72	0.72
2:F:228:VAL:C	2:F:230:MET:H	1.97	0.72
1:E:55:ASN:HB2	1:E:79:HIS:HB3	1.72	0.71
1:E:264:THR:O	1:E:265:PHE:HB3	1.89	0.71
2:F:47:MET:HE1	3:G:126:THR:O	1.90	0.71
1:I:80:VAL:HG23	1:I:127:LYS:O	1.89	0.71
1:I:144:HIS:HD1	1:I:163:TRP:CD1	2.07	0.71
1:I:195:ILE:HG22	1:I:196:TYR:N	2.05	0.71
1:I:264:THR:O	1:I:265:PHE:HB3	1.89	0.71
2:J:47:MET:HE1	3:K:126:THR:O	1.90	0.71
2:J:66:PRO:C	2:J:70:PRO:HG2	2.15	0.71
2:J:123:LEU:HG	2:J:124:VAL:HG13	1.72	0.71
1:A:177:VAL:HG22	1:A:178:THR:H	1.55	0.71
1:A:222:SER:CA	1:A:225:ARG:HB3	2.19	0.71
1:A:264:THR:O	1:A:265:PHE:HB3	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:55:PHE:O	2:F:124:VAL:HA	1.90	0.71
2:J:50:ALA:O	2:J:52:ASP:N	2.18	0.71
2:J:245:THR:O	2:J:247:LYS:N	2.17	0.71
1:A:144:HIS:HD1	1:A:163:TRP:CD1	2.07	0.71
2:B:184:SER:HB2	2:B:187:ASP:OD1	1.90	0.71
1:E:250:THR:HG21	2:F:134:LEU:HD12	1.70	0.71
2:F:66:PRO:C	2:F:70:PRO:HG2	2.15	0.71
2:F:203:ARG:HB3	2:F:207:ARG:NH2	2.05	0.71
2:J:238:PHE:HB2	2:J:241:LYS:CE	2.21	0.71
2:B:44:ILE:O	2:B:44:ILE:HD13	1.91	0.71
2:F:50:ALA:O	2:F:52:ASP:N	2.18	0.71
2:F:238:PHE:HB2	2:F:241:LYS:CE	2.21	0.71
1:I:66:LEU:HD13	1:I:70:GLU:O	1.89	0.71
2:J:30:PHE:HZ	4:L:511:UNK:HA	1.56	0.71
2:J:210:LEU:C	2:J:212:THR:H	1.98	0.71
3:K:107:LEU:CD2	3:K:168:ALA:HB2	2.21	0.71
1:A:206:ALA:O	1:A:210:ILE:HG13	1.91	0.71
3:C:88:ARG:CB	3:C:170:THR:HB	2.18	0.71
3:C:111:LEU:HD22	4:D:510:UNK:CB	2.20	0.71
1:E:222:SER:HA	1:E:225:ARG:HB3	1.73	0.71
1:I:177:VAL:HG22	1:I:178:THR:H	1.56	0.71
2:J:109:ARG:HG3	2:J:126:PRO:HD3	1.72	0.71
2:J:228:VAL:C	2:J:230:MET:H	1.97	0.71
3:K:111:LEU:HD22	4:L:510:UNK:CB	2.20	0.71
1:A:196:TYR:OH	2:B:121:ILE:HG21	1.91	0.71
1:A:247:LEU:O	1:A:251:ILE:HG22	1.90	0.71
1:E:105:LEU:HD23	1:E:137:ALA:CA	2.21	0.71
1:E:158:ILE:HG21	3:G:137:ILE:HD13	1.72	0.71
1:I:105:LEU:HD23	1:I:137:ALA:CA	2.20	0.71
2:J:91:PRO:HG3	2:J:141:LEU:HG	1.71	0.71
2:J:199:PRO:CG	3:K:138:ARG:HG3	2.20	0.71
3:K:169:LYS:HZ3	3:K:176:ALA:HA	1.55	0.71
2:F:13:PHE:HB3	2:F:19:ALA:HB2	1.71	0.71
2:F:91:PRO:HG3	2:F:141:LEU:HG	1.71	0.71
2:F:238:PHE:O	2:F:241:LYS:HG3	1.91	0.71
1:A:106:VAL:HG12	1:A:107:ARG:N	2.06	0.71
1:A:388:LEU:C	1:A:390:ASP:H	1.97	0.71
2:B:50:ALA:O	2:B:52:ASP:N	2.18	0.71
1:E:105:LEU:HD13	1:E:135:LEU:HD13	1.73	0.71
2:F:44:ILE:O	2:F:44:ILE:HD13	1.91	0.71
2:F:109:ARG:HG3	2:F:126:PRO:HD3	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:196:TYR:OH	2:J:121:ILE:HG21	1.91	0.71
2:F:142:LEU:H	2:F:142:LEU:CD1	2.04	0.71
1:E:224:LEU:C	1:E:226:ILE:H	1.99	0.71
1:E:247:LEU:O	1:E:251:ILE:HG22	1.90	0.71
1:E:399:ILE:HG12	1:E:400:GLY:N	2.04	0.71
2:F:184:SER:HB2	2:F:187:ASP:OD1	1.90	0.71
1:I:224:LEU:C	1:I:226:ILE:H	1.99	0.71
2:J:44:ILE:O	2:J:44:ILE:HD13	1.91	0.71
2:B:109:ARG:HG3	2:B:126:PRO:HD3	1.72	0.70
2:J:44:ILE:HG12	3:K:126:THR:HG21	1.71	0.70
2:J:55:PHE:O	2:J:124:VAL:HA	1.90	0.70
2:J:120:PRO:C	2:J:122:SER:H	1.96	0.70
1:A:105:LEU:HD23	1:A:137:ALA:CA	2.20	0.70
1:A:264:THR:O	1:A:264:THR:HG22	1.91	0.70
1:E:177:VAL:HG22	1:E:178:THR:H	1.55	0.70
1:I:98:ALA:HB1	1:I:100:GLU:HG3	1.74	0.70
2:J:142:LEU:H	2:J:142:LEU:CD1	2.03	0.70
1:A:105:LEU:HD13	1:A:135:LEU:HD13	1.73	0.70
1:A:265:PHE:CD1	1:A:268:THR:HB	2.27	0.70
2:B:123:LEU:HG	2:B:124:VAL:HG13	1.72	0.70
2:B:128:ALA:N	2:B:165:ASN:HD21	1.89	0.70
2:B:238:PHE:HB2	2:B:241:LYS:CE	2.21	0.70
1:E:80:VAL:HG23	1:E:127:LYS:O	1.89	0.70
1:I:206:ALA:O	1:I:210:ILE:HG13	1.91	0.70
2:B:34:LEU:HD13	2:B:84:PHE:CE1	2.27	0.70
3:C:74:LEU:O	3:C:78:LEU:HG	1.91	0.70
3:C:112:VAL:O	3:C:115:ALA:HB3	1.91	0.70
1:E:226:ILE:HD13	1:E:231:ASP:HB2	1.73	0.70
2:F:128:ALA:N	2:F:165:ASN:HD21	1.89	0.70
1:I:158:ILE:HG21	3:K:137:ILE:HD13	1.72	0.70
1:E:195:ILE:HG22	1:E:196:TYR:N	2.05	0.70
1:E:196:TYR:OH	2:F:121:ILE:HG21	1.91	0.70
1:E:388:LEU:C	1:E:390:ASP:H	1.97	0.70
3:G:74:LEU:O	3:G:78:LEU:HG	1.91	0.70
2:B:13:PHE:HB3	2:B:19:ALA:HB2	1.71	0.70
1:A:158:ILE:HG21	3:C:137:ILE:HD13	1.72	0.70
1:E:72:MET:HG2	1:E:73:VAL:N	2.07	0.70
2:F:238:PHE:HA	2:F:241:LYS:HE3	1.73	0.70
2:J:184:SER:HB2	2:J:187:ASP:OD1	1.90	0.70
2:J:238:PHE:HA	2:J:241:LYS:HE3	1.73	0.70
3:K:74:LEU:O	3:K:78:LEU:HG	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:VAL:HG11	1:A:143:TRP:CZ2	2.27	0.70
3:C:107:LEU:CD2	3:C:168:ALA:HB2	2.21	0.70
1:E:63:LYS:HG3	1:E:65:SER:H	1.54	0.70
2:F:75:THR:HG23	2:F:75:THR:O	1.89	0.70
1:I:265:PHE:CD1	1:I:268:THR:HB	2.27	0.70
2:J:203:ARG:HB3	2:J:207:ARG:NH2	2.05	0.70
2:J:238:PHE:O	2:J:241:LYS:HG3	1.91	0.70
2:B:75:THR:HG23	2:B:75:THR:O	1.89	0.70
1:E:98:ALA:HB1	1:E:100:GLU:HG3	1.74	0.70
3:G:107:LEU:CD2	3:G:168:ALA:HB2	2.21	0.70
1:I:264:THR:O	1:I:264:THR:HG22	1.91	0.70
2:J:34:LEU:HD13	2:J:84:PHE:CE1	2.27	0.70
2:J:184:SER:O	2:J:185:LEU:C	2.35	0.70
3:C:152:MET:C	3:C:156:ILE:HG13	2.17	0.70
1:E:206:ALA:O	1:E:210:ILE:HG13	1.91	0.70
3:K:112:VAL:O	3:K:115:ALA:HB3	1.91	0.70
1:A:42:GLU:HA	1:A:45:GLN:NE2	2.07	0.69
2:B:30:PHE:HZ	4:D:511:UNK:HA	1.56	0.69
2:B:161:PHE:O	2:B:164:ASN:HB3	1.92	0.69
1:E:247:LEU:HD21	2:F:135:TRP:CD1	2.27	0.69
1:E:270:PRO:C	1:E:271:LEU:HD23	2.17	0.69
1:E:304:TYR:CZ	1:E:423:PRO:HB3	2.27	0.69
2:F:34:LEU:HD13	2:F:84:PHE:CE1	2.27	0.69
3:G:118:ILE:HG12	3:G:157:TYR:CE2	2.27	0.69
1:I:55:ASN:HB2	1:I:79:HIS:HB3	1.73	0.69
1:I:247:LEU:O	1:I:251:ILE:HG22	1.90	0.69
1:I:304:TYR:HB3	1:I:311:LEU:HG	1.74	0.69
1:A:55:ASN:HB2	1:A:79:HIS:HB3	1.73	0.69
1:A:266:PRO:HD2	1:A:267:ARG:H	1.57	0.69
1:A:270:PRO:C	1:A:271:LEU:HD23	2.17	0.69
1:A:335:LEU:HD23	1:A:353:LEU:O	1.92	0.69
1:E:404:MET:HE2	1:E:404:MET:HA	1.74	0.69
2:F:184:SER:O	2:F:185:LEU:C	2.35	0.69
1:I:104:VAL:HG11	1:I:143:TRP:CZ2	2.27	0.69
1:I:404:MET:HE2	1:I:404:MET:HA	1.74	0.69
3:K:85:TRP:C	3:K:87:THR:H	2.01	0.69
1:A:224:LEU:C	1:A:226:ILE:H	1.99	0.69
1:A:226:ILE:HD13	1:A:231:ASP:HB2	1.73	0.69
2:B:238:PHE:O	2:B:241:LYS:HG3	1.91	0.69
1:I:106:VAL:HG12	1:I:107:ARG:N	2.06	0.69
1:E:104:VAL:HG11	1:E:143:TRP:CZ2	2.27	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:335:LEU:HD23	1:I:353:LEU:O	1.92	0.69
1:A:329:GLU:HG2	1:A:330:TYR:N	2.05	0.69
1:E:264:THR:O	1:E:264:THR:HG22	1.91	0.69
2:F:140:MET:HE1	2:F:144:GLY:CA	2.22	0.69
2:F:210:LEU:C	2:F:212:THR:H	1.98	0.69
1:I:247:LEU:HD21	2:J:135:TRP:CD1	2.27	0.69
2:B:142:LEU:H	2:B:142:LEU:CD1	2.04	0.69
1:E:265:PHE:CD1	1:E:268:THR:HB	2.27	0.69
1:E:364:THR:HG22	1:E:372:LYS:NZ	2.08	0.69
2:F:30:PHE:HZ	4:H:511:UNK:HA	1.56	0.69
2:F:211:ARG:HH22	3:G:158:SER:CA	2.05	0.69
3:G:112:VAL:O	3:G:115:ALA:HB3	1.91	0.69
1:I:42:GLU:HA	1:I:45:GLN:NE2	2.07	0.69
1:I:304:TYR:CZ	1:I:423:PRO:HB3	2.27	0.69
1:A:48:PHE:C	1:A:48:PHE:CD2	2.71	0.69
1:A:98:ALA:HB1	1:A:100:GLU:HG3	1.74	0.69
1:A:222:SER:HA	1:A:225:ARG:HB3	1.73	0.69
2:B:238:PHE:HA	2:B:241:LYS:HE3	1.73	0.69
3:C:118:ILE:HG12	3:C:157:TYR:CE2	2.27	0.69
1:E:393:TYR:CD1	2:J:249:ILE:HD13	2.28	0.69
3:G:85:TRP:C	3:G:87:THR:H	2.01	0.69
1:I:222:SER:HA	1:I:225:ARG:HB3	1.73	0.69
1:A:72:MET:HG2	1:A:73:VAL:N	2.07	0.69
1:A:195:ILE:HG22	1:A:196:TYR:N	2.05	0.69
1:A:247:LEU:HD21	2:B:135:TRP:CD1	2.27	0.69
2:B:33:LEU:HG	3:C:111:LEU:O	1.93	0.69
2:B:184:SER:O	2:B:185:LEU:C	2.35	0.69
3:C:50:GLY:HA2	3:C:58:PHE:HD2	1.58	0.69
3:C:85:TRP:C	3:C:87:THR:H	2.01	0.69
1:E:42:GLU:HA	1:E:45:GLN:NE2	2.07	0.69
1:E:271:LEU:HD21	2:F:173:HIS:NE2	2.08	0.69
2:F:198:MET:HA	2:F:198:MET:CE	2.22	0.69
1:I:271:LEU:HD21	2:J:173:HIS:NE2	2.08	0.69
2:J:140:MET:HE1	2:J:144:GLY:CA	2.22	0.69
2:J:229:SER:C	2:J:231:MET:N	2.48	0.69
2:J:244:SER:CA	2:J:247:LYS:HZ2	2.06	0.69
1:E:387:ARG:O	1:E:388:LEU:HD23	1.93	0.69
2:F:161:PHE:O	2:F:164:ASN:HB3	1.92	0.69
2:F:217:VAL:O	2:F:218:VAL:HG13	1.93	0.69
1:I:270:PRO:C	1:I:271:LEU:HD23	2.18	0.69
1:I:387:ARG:O	1:I:388:LEU:HD23	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:152:MET:C	3:K:156:ILE:HG13	2.17	0.69
1:A:387:ARG:O	1:A:388:LEU:HD23	1.93	0.68
2:B:210:LEU:C	2:B:212:THR:H	1.98	0.68
1:E:335:LEU:HD23	1:E:353:LEU:O	1.92	0.68
3:G:62:TRP:C	3:G:64:SER:H	2.01	0.68
1:I:226:ILE:HD13	1:I:231:ASP:HB2	1.73	0.68
2:J:33:LEU:HG	3:K:111:LEU:O	1.93	0.68
1:A:90:ASN:C	1:A:92:LYS:H	2.01	0.68
2:F:210:LEU:C	2:F:212:THR:N	2.44	0.68
1:I:72:MET:HG2	1:I:73:VAL:N	2.07	0.68
1:I:105:LEU:HD13	1:I:135:LEU:HD13	1.73	0.68
1:I:305:LYS:HG3	1:I:309:ARG:H	1.58	0.68
2:J:161:PHE:O	2:J:164:ASN:HB3	1.92	0.68
3:K:118:ILE:HG12	3:K:157:TYR:CE2	2.27	0.68
2:B:211:ARG:HH22	3:C:158:SER:CA	2.06	0.68
1:E:48:PHE:C	1:E:48:PHE:CD2	2.71	0.68
3:K:88:ARG:CB	3:K:170:THR:HB	2.18	0.68
1:I:266:PRO:HD2	1:I:267:ARG:H	1.57	0.68
1:I:364:THR:HG22	1:I:372:LYS:NZ	2.08	0.68
2:B:240:GLY:O	2:B:243:TYR:HB3	1.94	0.68
3:C:173:PRO:HG2	3:C:174:TYR:H	1.59	0.68
1:E:222:SER:C	1:E:225:ARG:HB3	2.19	0.68
2:F:33:LEU:HG	3:G:111:LEU:O	1.93	0.68
2:J:198:MET:HA	2:J:198:MET:CE	2.22	0.68
1:A:271:LEU:HD21	2:B:173:HIS:NE2	2.08	0.68
2:B:209:THR:O	2:B:211:ARG:N	2.26	0.68
2:F:238:PHE:CE1	2:F:242:TRP:HB2	2.29	0.68
2:J:240:GLY:O	2:J:243:TYR:HB3	1.94	0.68
3:G:66:LEU:C	3:G:68:THR:H	2.01	0.68
3:G:88:ARG:CB	3:G:170:THR:HB	2.18	0.68
3:G:152:MET:C	3:G:156:ILE:HG13	2.17	0.68
3:K:50:GLY:HA2	3:K:58:PHE:HD2	1.58	0.68
3:K:131:THR:O	3:K:135:THR:HG23	1.94	0.68
1:A:222:SER:C	1:A:225:ARG:HB3	2.19	0.68
1:A:304:TYR:CZ	1:A:423:PRO:HB3	2.27	0.68
2:F:209:THR:O	2:F:211:ARG:N	2.26	0.68
1:I:222:SER:C	1:I:225:ARG:HB3	2.19	0.68
2:J:210:LEU:C	2:J:212:THR:N	2.45	0.68
1:A:364:THR:HG22	1:A:372:LYS:NZ	2.08	0.68
1:E:90:ASN:C	1:E:92:LYS:H	2.01	0.68
1:E:106:VAL:HG12	1:E:107:ARG:N	2.06	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:304:TYR:HB3	1:E:311:LEU:HG	1.74	0.68
1:I:90:ASN:C	1:I:92:LYS:H	2.00	0.68
2:J:131:VAL:HB	2:J:132:PRO:CD	2.24	0.68
3:C:66:LEU:C	3:C:68:THR:H	2.01	0.68
2:F:205:VAL:HG22	2:J:239:VAL:O	1.94	0.68
2:F:240:GLY:O	2:F:243:TYR:HB3	1.94	0.68
3:G:114:TYR:CZ	3:G:118:ILE:HD11	2.29	0.68
1:I:406:PHE:CD1	1:I:412:ARG:HB3	2.29	0.68
2:J:211:ARG:HH22	3:K:158:SER:CA	2.05	0.68
3:K:173:PRO:HG2	3:K:174:TYR:H	1.59	0.68
1:A:304:TYR:HB3	1:A:311:LEU:HG	1.74	0.67
2:B:238:PHE:CE1	2:B:242:TRP:HB2	2.29	0.67
2:F:128:ALA:HB3	2:F:164:ASN:OD1	1.95	0.67
2:J:52:ASP:HB3	2:J:55:PHE:HB2	1.76	0.67
2:J:217:VAL:O	2:J:218:VAL:HG13	1.93	0.67
2:J:238:PHE:HD1	2:J:241:LYS:HB2	1.58	0.67
2:J:238:PHE:CE1	2:J:242:TRP:HB2	2.29	0.67
3:K:66:LEU:C	3:K:68:THR:H	2.01	0.67
1:A:202:TRP:HZ3	1:A:250:THR:HG23	1.59	0.67
2:F:52:ASP:HB3	2:F:55:PHE:HB2	1.76	0.67
2:F:140:MET:CE	2:F:144:GLY:HA2	2.23	0.67
2:F:244:SER:HA	2:F:247:LYS:NZ	2.09	0.67
3:G:50:GLY:HA2	3:G:58:PHE:HD2	1.58	0.67
3:G:173:PRO:HG2	3:G:174:TYR:H	1.59	0.67
1:I:407:SER:H	1:I:411:LYS:H	1.42	0.67
1:A:308:GLY:O	1:A:309:ARG:HG3	1.95	0.67
1:E:266:PRO:HD2	1:E:267:ARG:H	1.57	0.67
1:E:306:VAL:HB	1:E:425:PHE:HA	1.77	0.67
1:E:406:PHE:CD1	1:E:412:ARG:HB3	2.29	0.67
3:G:131:THR:O	3:G:135:THR:HG23	1.94	0.67
2:J:65:TRP:C	2:J:67:THR:H	2.03	0.67
2:B:65:TRP:C	2:B:67:THR:H	2.03	0.67
1:E:308:GLY:O	1:E:309:ARG:HG3	1.95	0.67
2:F:155:LEU:HD23	2:F:237:TRP:HH2	1.60	0.67
2:F:237:TRP:HE3	2:F:237:TRP:C	2.02	0.67
1:A:276:GLN:C	1:A:278:PRO:HD2	2.20	0.67
1:A:330:TYR:O	1:A:337:PHE:HB2	1.95	0.67
2:B:217:VAL:O	2:B:218:VAL:HG13	1.93	0.67
1:E:148:GLN:HB2	1:E:158:ILE:HA	1.77	0.67
1:E:276:GLN:C	1:E:278:PRO:HD2	2.19	0.67
1:I:48:PHE:C	1:I:48:PHE:CD2	2.71	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:114:TYR:CZ	3:K:118:ILE:HD11	2.29	0.67
2:B:52:ASP:HB3	2:B:55:PHE:HB2	1.76	0.67
1:E:305:LYS:HG3	1:E:309:ARG:H	1.58	0.67
1:E:407:SER:H	1:E:411:LYS:H	1.43	0.67
2:J:209:THR:O	2:J:211:ARG:N	2.26	0.67
3:K:62:TRP:C	3:K:64:SER:H	2.01	0.67
2:B:237:TRP:C	2:B:237:TRP:HE3	2.02	0.67
3:G:169:LYS:HZ3	3:G:176:ALA:HA	1.59	0.67
1:I:219:ILE:HG13	2:J:27:ASP:OD2	1.95	0.67
1:A:406:PHE:CD1	1:A:412:ARG:HB3	2.29	0.67
1:E:219:ILE:HG13	2:F:27:ASP:OD2	1.95	0.67
2:F:65:TRP:C	2:F:67:THR:H	2.03	0.67
2:B:198:MET:HA	2:B:198:MET:CE	2.21	0.67
2:B:238:PHE:HD1	2:B:241:LYS:HB2	1.59	0.67
3:C:114:TYR:CZ	3:C:118:ILE:HD11	2.29	0.67
1:I:202:TRP:HZ3	1:I:250:THR:HG23	1.59	0.67
2:J:128:ALA:HB3	2:J:164:ASN:OD1	1.95	0.67
2:B:205:VAL:HG22	2:F:239:VAL:HG12	1.76	0.67
1:I:276:GLN:C	1:I:278:PRO:HD2	2.20	0.67
1:A:261:THR:HG22	2:B:170:ALA:HB3	1.77	0.66
1:A:305:LYS:HG3	1:A:309:ARG:H	1.58	0.66
1:A:404:MET:HE2	1:A:404:MET:HA	1.74	0.66
1:A:407:SER:H	1:A:411:LYS:H	1.42	0.66
3:C:62:TRP:C	3:C:64:SER:H	2.01	0.66
2:F:90:LEU:C	2:F:92:PHE:H	2.03	0.66
2:F:238:PHE:HD1	2:F:241:LYS:HB2	1.59	0.66
1:I:330:TYR:O	1:I:337:PHE:HB2	1.95	0.66
1:A:148:GLN:HB2	1:A:158:ILE:HA	1.77	0.66
2:B:90:LEU:C	2:B:92:PHE:H	2.03	0.66
1:I:308:GLY:O	1:I:309:ARG:HG3	1.95	0.66
1:I:361:THR:HG22	1:I:362:ASP:N	2.10	0.66
2:J:90:LEU:C	2:J:92:PHE:H	2.03	0.66
1:A:219:ILE:HG13	2:B:27:ASP:OD2	1.95	0.66
2:B:244:SER:HA	2:B:247:LYS:NZ	2.09	0.66
1:E:223:TYR:O	1:E:226:ILE:HB	1.96	0.66
1:I:336:ARG:O	1:I:355:ALA:HB3	1.95	0.66
1:A:223:TYR:O	1:A:226:ILE:HB	1.96	0.66
1:A:306:VAL:HB	1:A:425:PHE:HA	1.77	0.66
1:A:309:ARG:HB3	1:A:380:ASP:O	1.96	0.66
2:F:120:PRO:C	2:F:122:SER:N	2.51	0.66
2:F:235:LEU:O	2:F:238:PHE:HB3	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:306:VAL:HB	1:I:425:PHE:HA	1.77	0.66
2:J:237:TRP:C	2:J:237:TRP:HE3	2.02	0.66
2:B:235:LEU:O	2:B:238:PHE:HB3	1.96	0.66
2:B:244:SER:CA	2:B:247:LYS:HZ2	2.06	0.66
3:C:131:THR:O	3:C:135:THR:HG23	1.94	0.66
1:E:261:THR:HG22	2:F:170:ALA:HB3	1.77	0.66
2:J:140:MET:CE	2:J:144:GLY:HA2	2.23	0.66
2:B:140:MET:CE	2:B:144:GLY:HA2	2.23	0.66
2:B:155:LEU:HD23	2:B:237:TRP:HH2	1.60	0.66
2:B:176:THR:CG2	2:B:178:GLN:HE22	2.09	0.66
1:I:223:TYR:O	1:I:226:ILE:HB	1.96	0.66
2:J:235:LEU:O	2:J:238:PHE:HB3	1.96	0.66
2:B:128:ALA:HB3	2:B:164:ASN:OD1	1.95	0.66
1:E:422:ILE:HD12	1:E:422:ILE:N	2.11	0.66
2:J:88:PHE:O	2:J:90:LEU:N	2.29	0.66
2:J:176:THR:CG2	2:J:178:GLN:HE22	2.09	0.66
1:A:233:GLU:CD	1:A:233:GLU:H	2.03	0.66
2:B:243:TYR:C	2:B:245:THR:N	2.52	0.66
1:E:247:LEU:HD13	1:E:247:LEU:C	2.21	0.66
1:I:366:LEU:HD13	1:I:372:LYS:HD2	1.78	0.66
2:J:128:ALA:N	2:J:165:ASN:HD21	1.89	0.66
2:B:86:GLU:HG3	2:B:87:ASN:OD1	1.96	0.66
2:B:121:ILE:HD12	2:B:121:ILE:N	2.02	0.66
1:E:96:LEU:HA	1:E:149:ILE:HA	1.78	0.66
1:E:309:ARG:HB3	1:E:380:ASP:O	1.96	0.66
2:F:32:THR:O	2:F:33:LEU:C	2.39	0.66
2:F:114:TRP:O	2:F:118:TYR:HA	1.96	0.66
2:F:131:VAL:HB	2:F:132:PRO:CD	2.24	0.66
1:A:96:LEU:HA	1:A:149:ILE:HA	1.78	0.66
2:B:98:VAL:O	2:B:99:SER:C	2.39	0.66
3:G:99:GLU:O	3:G:103:ARG:HG3	1.96	0.66
1:I:233:GLU:CD	1:I:233:GLU:H	2.03	0.66
2:J:91:PRO:CB	2:J:141:LEU:HG	2.26	0.66
2:J:120:PRO:C	2:J:122:SER:N	2.51	0.66
2:J:142:LEU:HD12	2:J:142:LEU:N	2.09	0.66
3:K:45:TYR:HB3	3:K:61:TYR:O	1.96	0.66
2:B:21:GLY:O	2:B:23:VAL:N	2.24	0.65
2:B:88:PHE:O	2:B:90:LEU:N	2.29	0.65
2:J:65:TRP:CB	2:J:66:PRO:HD3	2.26	0.65
2:J:98:VAL:O	2:J:99:SER:C	2.39	0.65
2:B:131:VAL:HB	2:B:132:PRO:CD	2.24	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:204:ILE:C	1:E:206:ALA:N	2.45	0.65
1:E:336:ARG:O	1:E:355:ALA:HB3	1.95	0.65
1:E:366:LEU:HD13	1:E:372:LYS:HD2	1.78	0.65
1:I:247:LEU:C	1:I:247:LEU:HD13	2.21	0.65
2:J:86:GLU:HG3	2:J:87:ASN:OD1	1.96	0.65
2:J:114:TRP:O	2:J:118:TYR:HA	1.96	0.65
2:J:155:LEU:HD23	2:J:237:TRP:HH2	1.60	0.65
3:K:76:SER:HB3	3:K:159:ILE:HD13	1.79	0.65
1:E:43:LYS:N	1:E:50:ARG:HH22	1.95	0.65
1:E:330:TYR:O	1:E:337:PHE:HB2	1.95	0.65
2:F:204:MET:SD	2:F:207:ARG:HD2	2.37	0.65
1:I:309:ARG:HB3	1:I:380:ASP:O	1.96	0.65
1:A:58:ASP:O	1:A:76:GLY:HA2	1.97	0.65
3:C:140:THR:C	3:C:142:PHE:H	2.03	0.65
3:C:153:SER:O	3:C:156:ILE:HB	1.97	0.65
1:E:43:LYS:H	1:E:50:ARG:NH2	1.95	0.65
1:I:43:LYS:N	1:I:50:ARG:HH22	1.95	0.65
1:I:235:ILE:HD11	2:J:89:LYS:HD2	1.79	0.65
2:J:14:HIS:HB2	3:K:98:ARG:NH2	2.12	0.65
3:K:22:ARG:HB3	3:K:22:ARG:HH11	1.60	0.65
1:A:42:GLU:HA	1:A:45:GLN:HE21	1.61	0.65
1:A:336:ARG:O	1:A:355:ALA:HB3	1.95	0.65
2:B:114:TRP:O	2:B:118:TYR:HA	1.96	0.65
2:F:14:HIS:HB2	3:G:98:ARG:NH2	2.12	0.65
1:I:116:PHE:CE2	2:J:179:HIS:HB2	2.32	0.65
1:I:148:GLN:HB2	1:I:158:ILE:HA	1.77	0.65
1:A:247:LEU:HD21	2:B:135:TRP:HD1	1.61	0.65
2:B:65:TRP:CB	2:B:66:PRO:HD3	2.26	0.65
2:B:204:MET:SD	2:B:207:ARG:HD2	2.36	0.65
2:F:91:PRO:CB	2:F:141:LEU:HG	2.26	0.65
2:F:176:THR:CG2	2:F:178:GLN:HE22	2.09	0.65
3:G:45:TYR:HB3	3:G:61:TYR:O	1.95	0.65
1:I:43:LYS:H	1:I:50:ARG:NH2	1.95	0.65
1:I:103:PRO:HG3	2:J:194:VAL:O	1.97	0.65
2:J:204:MET:SD	2:J:207:ARG:HD2	2.37	0.65
2:B:91:PRO:CB	2:B:141:LEU:HG	2.26	0.65
2:F:65:TRP:CB	2:F:66:PRO:HD3	2.26	0.65
2:J:66:PRO:O	2:J:70:PRO:HG2	1.97	0.65
2:J:245:THR:C	2:J:247:LYS:H	2.05	0.65
2:B:14:HIS:HB2	3:C:98:ARG:NH2	2.12	0.65
3:C:45:TYR:HB3	3:C:61:TYR:O	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:202:TRP:HZ3	1:E:250:THR:HG23	1.60	0.65
2:F:98:VAL:O	2:F:99:SER:C	2.39	0.65
2:F:121:ILE:HD12	2:F:121:ILE:N	2.02	0.65
3:G:106:VAL:HB	3:G:167:TYR:OH	1.97	0.65
3:G:153:SER:O	3:G:156:ILE:HB	1.97	0.65
1:I:231:ASP:HA	1:I:233:GLU:OE2	1.97	0.65
1:I:247:LEU:HD21	2:J:135:TRP:HD1	1.61	0.65
1:A:201:PRO:HA	1:A:204:ILE:CG1	2.27	0.65
1:A:204:ILE:C	1:A:206:ALA:N	2.45	0.65
1:A:247:LEU:HB2	2:B:138:ILE:HD13	1.78	0.65
3:C:106:VAL:HB	3:C:167:TYR:OH	1.97	0.65
1:E:201:PRO:HA	1:E:204:ILE:CG1	2.27	0.65
1:A:150:ASN:CG	1:A:156:PRO:HA	2.22	0.65
1:A:247:LEU:C	1:A:247:LEU:HD13	2.21	0.65
3:C:76:SER:HB3	3:C:159:ILE:HD13	1.79	0.65
1:E:116:PHE:CE2	2:F:179:HIS:HB2	2.32	0.65
2:F:86:GLU:HG3	2:F:87:ASN:OD1	1.96	0.65
1:I:150:ASN:CG	1:I:156:PRO:HA	2.22	0.65
1:I:261:THR:HG22	2:J:170:ALA:HB3	1.77	0.65
1:I:295:VAL:HG11	1:I:405:PHE:HD2	1.62	0.65
1:I:422:ILE:N	1:I:422:ILE:HD12	2.11	0.65
1:A:235:ILE:HD11	2:B:89:LYS:HD2	1.79	0.64
2:B:32:THR:O	2:B:33:LEU:C	2.39	0.64
2:F:88:PHE:O	2:F:90:LEU:N	2.29	0.64
3:G:22:ARG:HB3	3:G:22:ARG:HH11	1.60	0.64
2:J:249:ILE:O	2:J:249:ILE:HG22	1.97	0.64
3:K:99:GLU:O	3:K:103:ARG:HG3	1.96	0.64
3:K:153:SER:O	3:K:156:ILE:HB	1.97	0.64
1:A:422:ILE:HD12	1:A:422:ILE:N	2.11	0.64
3:C:99:GLU:O	3:C:103:ARG:HG3	1.96	0.64
2:F:14:HIS:HB2	3:G:98:ARG:HH22	1.62	0.64
2:F:199:PRO:HD3	3:G:133:HIS:CG	2.32	0.64
2:J:32:THR:O	2:J:33:LEU:C	2.39	0.64
1:A:43:LYS:H	1:A:50:ARG:NH2	1.95	0.64
1:A:43:LYS:N	1:A:50:ARG:HH22	1.95	0.64
1:A:204:ILE:O	1:A:206:ALA:N	2.31	0.64
1:E:233:GLU:H	1:E:233:GLU:CD	2.03	0.64
1:E:247:LEU:HB2	2:F:138:ILE:HD13	1.78	0.64
1:I:58:ASP:O	1:I:76:GLY:HA2	1.97	0.64
1:A:116:PHE:CE2	2:B:179:HIS:HB2	2.32	0.64
1:A:231:ASP:HA	1:A:233:GLU:OE2	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:210:ILE:HA	2:F:92:PHE:CZ	2.32	0.64
3:G:76:SER:HB3	3:G:159:ILE:HD13	1.79	0.64
1:I:247:LEU:HB2	2:J:138:ILE:HD13	1.78	0.64
2:J:109:ARG:HG2	2:J:109:ARG:HH11	1.63	0.64
2:B:140:MET:HE1	2:B:144:GLY:CA	2.22	0.64
2:B:212:THR:O	2:B:214:GLY:N	2.30	0.64
2:B:229:SER:C	2:B:231:MET:N	2.48	0.64
1:E:103:PRO:HG3	2:F:194:VAL:O	1.97	0.64
2:F:88:PHE:O	2:F:89:LYS:C	2.41	0.64
2:J:155:LEU:HD13	2:J:159:LEU:CD1	2.28	0.64
2:J:199:PRO:HD3	3:K:133:HIS:CG	2.32	0.64
2:J:212:THR:O	2:J:214:GLY:N	2.30	0.64
1:A:103:PRO:HG3	2:B:194:VAL:O	1.97	0.64
1:E:231:ASP:HA	1:E:233:GLU:OE2	1.97	0.64
2:F:249:ILE:O	2:F:249:ILE:HG22	1.98	0.64
3:G:107:LEU:HD23	3:G:168:ALA:HB2	1.80	0.64
3:G:110:TRP:HB3	3:G:164:ALA:HB2	1.80	0.64
1:I:373:THR:HG22	1:I:373:THR:O	1.98	0.64
2:J:121:ILE:HD12	2:J:121:ILE:N	2.03	0.64
2:J:244:SER:HA	2:J:247:LYS:NZ	2.09	0.64
1:A:210:ILE:HA	2:B:92:PHE:CZ	2.32	0.64
1:A:333:ALA:C	1:A:335:LEU:H	2.05	0.64
3:C:50:GLY:HA2	3:C:58:PHE:CD2	2.33	0.64
1:E:269:ILE:HB	1:E:270:PRO:CD	2.28	0.64
1:E:333:ALA:C	1:E:335:LEU:H	2.05	0.64
2:F:155:LEU:HD13	2:F:159:LEU:CD1	2.28	0.64
1:I:210:ILE:HA	2:J:92:PHE:CZ	2.32	0.64
3:K:110:TRP:HB3	3:K:164:ALA:HB2	1.80	0.64
1:A:163:TRP:CD1	1:A:163:TRP:H	2.16	0.64
2:B:239:VAL:CG1	2:J:205:VAL:HA	2.27	0.64
2:F:204:MET:C	2:J:239:VAL:HG11	2.23	0.64
3:G:140:THR:C	3:G:142:PHE:H	2.03	0.64
1:I:374:ILE:HD12	1:I:375:GLU:H	1.63	0.64
2:J:14:HIS:HB2	3:K:98:ARG:HH22	1.62	0.64
3:K:102:ARG:HG2	3:K:102:ARG:HH11	1.63	0.64
3:K:106:VAL:HB	3:K:167:TYR:OH	1.97	0.64
2:B:205:VAL:O	2:B:209:THR:HB	1.98	0.64
3:C:107:LEU:HD23	3:C:168:ALA:HB2	1.80	0.64
1:E:163:TRP:CD1	1:E:163:TRP:H	2.16	0.64
2:F:205:VAL:O	2:F:209:THR:HB	1.98	0.64
3:G:104:HIS:C	3:G:106:VAL:N	2.53	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:42:GLU:HA	1:I:45:GLN:HE21	1.61	0.64
1:I:174:LYS:O	1:I:176:PRO:HD3	1.98	0.64
3:K:107:LEU:HD23	3:K:168:ALA:HB2	1.80	0.64
3:K:140:THR:C	3:K:142:PHE:H	2.03	0.64
1:A:366:LEU:HD13	1:A:372:LYS:HD2	1.78	0.64
3:C:22:ARG:HB3	3:C:22:ARG:HH11	1.60	0.64
1:E:58:ASP:O	1:E:76:GLY:HA2	1.97	0.64
2:F:109:ARG:HG2	2:F:109:ARG:HH11	1.63	0.64
2:F:231:MET:O	2:F:232:VAL:C	2.41	0.64
1:I:278:PRO:O	1:I:279:LEU:HB2	1.98	0.64
3:K:50:GLY:HA2	3:K:58:PHE:CD2	2.33	0.64
3:C:102:ARG:HG2	3:C:102:ARG:HH11	1.63	0.63
2:F:140:MET:HA	2:F:140:MET:HE2	1.80	0.63
1:I:96:LEU:HA	1:I:149:ILE:HA	1.78	0.63
1:I:204:ILE:O	1:I:206:ALA:N	2.31	0.63
2:J:140:MET:HE2	2:J:140:MET:HA	1.80	0.63
1:A:66:LEU:O	1:A:166:ILE:HA	1.98	0.63
1:E:235:ILE:HD11	2:F:89:LYS:HD2	1.79	0.63
1:E:247:LEU:HD21	2:F:135:TRP:HD1	1.61	0.63
1:E:295:VAL:HG11	1:E:405:PHE:HD2	1.62	0.63
2:F:212:THR:O	2:F:214:GLY:N	2.30	0.63
1:I:201:PRO:HA	1:I:204:ILE:CG1	2.27	0.63
2:B:88:PHE:O	2:B:89:LYS:C	2.41	0.63
2:B:155:LEU:HD13	2:B:159:LEU:CD1	2.28	0.63
2:B:199:PRO:HD3	3:C:133:HIS:CG	2.32	0.63
1:E:187:LEU:C	1:E:189:THR:H	2.07	0.63
1:E:204:ILE:O	1:E:206:ALA:N	2.31	0.63
2:F:148:ILE:HG13	2:F:149:THR:N	2.13	0.63
1:I:333:ALA:C	1:I:335:LEU:H	2.05	0.63
2:B:66:PRO:O	2:B:70:PRO:HG2	1.97	0.63
2:B:249:ILE:HG22	2:B:249:ILE:O	1.98	0.63
1:A:405:PHE:O	1:A:412:ARG:HA	1.98	0.63
2:B:82:ALA:HB3	2:B:231:MET:HG3	1.81	0.63
3:C:101:LEU:HD23	4:D:518:UNK:HA	1.81	0.63
1:E:66:LEU:O	1:E:166:ILE:HA	1.98	0.63
1:E:145:VAL:HG21	1:E:164:ILE:HD12	1.81	0.63
1:E:150:ASN:CG	1:E:156:PRO:HA	2.22	0.63
1:E:374:ILE:HD12	1:E:375:GLU:H	1.63	0.63
2:F:57:VAL:HA	2:F:60:LYS:CG	2.29	0.63
2:F:66:PRO:O	2:F:70:PRO:HG2	1.97	0.63
2:F:142:LEU:HD12	2:F:142:LEU:N	2.10	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:101:LEU:HD23	4:H:518:UNK:HA	1.81	0.63
1:I:187:LEU:C	1:I:189:THR:H	2.07	0.63
2:J:62:ARG:O	2:J:66:PRO:HD2	1.99	0.63
2:J:82:ALA:HB3	2:J:231:MET:HG3	1.81	0.63
2:J:231:MET:O	2:J:232:VAL:C	2.41	0.63
1:A:97:ASN:N	1:A:148:GLN:O	2.32	0.63
1:A:361:THR:HG22	1:A:362:ASP:N	2.10	0.63
1:A:374:ILE:HD12	1:A:375:GLU:H	1.63	0.63
2:B:14:HIS:HB2	3:C:98:ARG:HH22	1.62	0.63
2:J:57:VAL:HA	2:J:60:LYS:CG	2.29	0.63
2:J:148:ILE:HG13	2:J:149:THR:N	2.13	0.63
3:K:159:ILE:HA	3:K:162:VAL:HG22	1.80	0.63
1:A:269:ILE:HB	1:A:270:PRO:CD	2.28	0.63
1:A:295:VAL:HG11	1:A:405:PHE:HD2	1.62	0.63
2:B:13:PHE:HB3	2:B:19:ALA:CB	2.29	0.63
3:C:110:TRP:HB3	3:C:164:ALA:HB2	1.80	0.63
1:E:113:GLY:HA3	1:E:279:LEU:CD2	2.25	0.63
1:E:187:LEU:HD23	2:F:192:HIS:CD2	2.34	0.63
1:E:235:ILE:HG22	1:E:236:GLY:N	2.14	0.63
2:F:13:PHE:HB3	2:F:19:ALA:CB	2.29	0.63
2:F:245:THR:C	2:F:247:LYS:H	2.05	0.63
3:G:159:ILE:HA	3:G:162:VAL:HG22	1.80	0.63
1:A:187:LEU:C	1:A:189:THR:H	2.07	0.63
1:A:373:THR:HG22	1:A:373:THR:O	1.97	0.63
2:B:231:MET:O	2:B:232:VAL:C	2.41	0.63
1:E:174:LYS:O	1:E:176:PRO:HD3	1.98	0.63
1:E:373:THR:O	1:E:373:THR:HG22	1.97	0.63
1:E:383:TRP:O	1:E:388:LEU:HB2	1.99	0.63
3:G:102:ARG:HG2	3:G:102:ARG:HH11	1.63	0.63
3:G:132:TRP:NE1	3:G:143:THR:HB	2.12	0.63
1:A:174:LYS:O	1:A:176:PRO:HD3	1.98	0.63
2:B:57:VAL:HA	2:B:60:LYS:CG	2.29	0.63
2:F:176:THR:HG22	2:F:177:GLU:N	2.14	0.63
1:I:163:TRP:CD1	1:I:163:TRP:H	2.16	0.63
2:J:88:PHE:O	2:J:89:LYS:C	2.41	0.63
2:J:205:VAL:O	2:J:209:THR:HB	1.98	0.63
3:K:104:HIS:O	3:K:105:VAL:C	2.42	0.63
1:A:235:ILE:HG22	1:A:236:GLY:N	2.14	0.62
2:B:57:VAL:HA	2:B:60:LYS:HG3	1.81	0.62
3:C:159:ILE:O	3:C:160:MET:C	2.42	0.62
2:F:39:LEU:HD23	2:F:39:LEU:C	2.25	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:118:TYR:CE1	3:G:47:TRP:HH2	2.17	0.62
2:F:159:LEU:HG	2:F:247:LYS:NZ	2.14	0.62
1:I:108:THR:HB	1:I:134:ASP:HB3	1.81	0.62
2:J:39:LEU:HD23	2:J:39:LEU:C	2.24	0.62
3:K:101:LEU:HD23	4:L:518:UNK:HA	1.81	0.62
3:K:104:HIS:C	3:K:106:VAL:N	2.53	0.62
1:A:187:LEU:HD23	2:B:192:HIS:CD2	2.34	0.62
2:B:38:VAL:CG1	2:B:39:LEU:N	2.62	0.62
2:B:118:TYR:CE1	3:C:47:TRP:HH2	2.17	0.62
1:E:42:GLU:HA	1:E:45:GLN:HE21	1.61	0.62
2:F:34:LEU:HD13	2:F:84:PHE:HE1	1.64	0.62
3:G:50:GLY:HA2	3:G:58:PHE:CD2	2.33	0.62
1:I:66:LEU:O	1:I:166:ILE:HA	1.98	0.62
1:I:299:LEU:HD23	1:I:315:VAL:HG22	1.82	0.62
2:J:13:PHE:HB3	2:J:19:ALA:CB	2.29	0.62
2:J:21:GLY:O	2:J:23:VAL:N	2.24	0.62
2:B:142:LEU:HD12	2:B:142:LEU:N	2.10	0.62
2:F:172:LEU:H	2:F:172:LEU:HD12	1.64	0.62
1:I:111:PHE:O	1:I:131:PHE:HB2	1.99	0.62
1:A:111:PHE:O	1:A:131:PHE:HB2	1.99	0.62
3:C:159:ILE:HA	3:C:162:VAL:HG22	1.80	0.62
1:E:172:ASP:O	1:E:173:PHE:O	2.17	0.62
1:E:278:PRO:O	1:E:279:LEU:HB2	1.98	0.62
2:F:62:ARG:O	2:F:66:PRO:HD2	1.99	0.62
3:G:148:ILE:CA	3:G:152:MET:HB2	2.28	0.62
1:I:316:LYS:HE2	1:I:373:THR:HG23	1.81	0.62
1:I:405:PHE:O	1:I:412:ARG:HA	1.98	0.62
2:J:118:TYR:CE1	3:K:47:TRP:HH2	2.17	0.62
3:K:159:ILE:O	3:K:160:MET:C	2.42	0.62
3:C:104:HIS:O	3:C:105:VAL:C	2.42	0.62
1:E:238:ASP:O	1:E:242:VAL:HG23	2.00	0.62
1:E:295:VAL:N	1:E:413:TYR:CE2	2.67	0.62
1:E:299:LEU:HD23	1:E:315:VAL:HG22	1.82	0.62
2:F:83:PHE:CE2	4:H:507:UNK:CB	2.83	0.62
2:F:141:LEU:HB3	2:F:142:LEU:HD12	1.82	0.62
1:I:97:ASN:N	1:I:148:GLN:O	2.32	0.62
2:J:134:LEU:C	2:J:136:LEU:N	2.58	0.62
2:J:233:TYR:C	2:J:233:TYR:CD1	2.78	0.62
1:A:139:ARG:NH1	3:C:47:TRP:CZ2	2.68	0.62
1:A:172:ASP:O	1:A:173:PHE:O	2.17	0.62
1:A:331:THR:HA	1:A:335:LEU:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:132:TRP:NE1	3:C:143:THR:HB	2.12	0.62
3:C:148:ILE:CA	3:C:152:MET:HB2	2.28	0.62
1:E:405:PHE:O	1:E:412:ARG:HA	1.99	0.62
3:G:140:THR:HG22	3:G:141:ASP:H	1.65	0.62
1:I:68:VAL:HG11	1:I:172:ASP:HB2	1.82	0.62
1:I:269:ILE:HB	1:I:270:PRO:CD	2.28	0.62
3:K:65:ILE:HG12	5:O:7:UNK:CB	2.30	0.62
1:A:179:LEU:HD13	2:B:174:GLN:NE2	2.15	0.62
2:B:109:ARG:HG2	2:B:109:ARG:HH11	1.63	0.62
3:C:104:HIS:C	3:C:106:VAL:N	2.53	0.62
1:E:107:ARG:HG2	2:F:191:PHE:CD1	2.35	0.62
1:E:179:LEU:HD13	2:F:174:GLN:NE2	2.15	0.62
2:F:123:LEU:HD23	2:F:124:VAL:H	1.65	0.62
2:J:172:LEU:HD12	2:J:172:LEU:H	1.64	0.62
2:J:176:THR:HG22	2:J:177:GLU:N	2.14	0.62
2:J:233:TYR:O	2:J:234:PHE:C	2.43	0.62
1:A:145:VAL:HG21	1:A:164:ILE:HD12	1.81	0.62
1:A:295:VAL:N	1:A:413:TYR:CE2	2.67	0.62
2:B:123:LEU:HD23	2:B:124:VAL:H	1.65	0.62
2:B:166:TRP:CD2	2:B:170:ALA:HB2	2.35	0.62
2:B:233:TYR:CD1	2:B:233:TYR:C	2.78	0.62
1:E:297:ALA:HB3	1:E:416:GLU:O	2.00	0.62
3:G:159:ILE:O	3:G:160:MET:C	2.42	0.62
1:I:42:GLU:HA	1:I:45:GLN:HG3	1.82	0.62
1:I:139:ARG:NH1	3:K:47:TRP:CZ2	2.68	0.62
1:I:179:LEU:HD23	1:I:179:LEU:N	2.09	0.62
1:I:187:LEU:HD23	2:J:192:HIS:CD2	2.34	0.62
1:I:199:HIS:HE1	2:J:128:ALA:N	1.98	0.62
2:J:159:LEU:HG	2:J:247:LYS:NZ	2.14	0.62
2:J:245:THR:CG2	2:J:246:THR:N	2.61	0.62
3:K:148:ILE:CA	3:K:152:MET:HB2	2.28	0.62
5:O:19:UNK:O	5:O:23:UNK:CB	2.48	0.62
1:A:41:GLY:O	1:A:42:GLU:O	2.17	0.62
2:B:203:ARG:C	2:B:207:ARG:HE	2.08	0.62
1:E:199:HIS:HE1	2:F:128:ALA:N	1.98	0.62
1:E:422:ILE:HG12	2:J:177:GLU:HG3	1.82	0.62
5:N:19:UNK:O	5:N:23:UNK:CB	2.48	0.62
1:I:107:ARG:HG2	2:J:191:PHE:CD1	2.35	0.62
1:I:295:VAL:N	1:I:413:TYR:CE2	2.67	0.62
1:I:383:TRP:O	1:I:388:LEU:HB2	1.99	0.62
2:J:123:LEU:HD23	2:J:124:VAL:H	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:203:ARG:C	2:J:207:ARG:HE	2.08	0.62
1:A:68:VAL:HG11	1:A:172:ASP:HB2	1.82	0.62
1:A:265:PHE:CE1	1:A:268:THR:HB	2.35	0.62
1:A:316:LYS:HE2	1:A:373:THR:HG23	1.81	0.62
1:A:383:TRP:O	1:A:388:LEU:HB2	1.99	0.62
2:B:140:MET:HE2	2:B:140:MET:HA	1.80	0.62
1:E:41:GLY:O	1:E:42:GLU:O	2.17	0.62
1:E:42:GLU:HA	1:E:45:GLN:HG3	1.82	0.62
2:F:233:TYR:CD1	2:F:233:TYR:C	2.78	0.62
1:I:48:PHE:CB	1:I:394:ASP:HB3	2.29	0.62
3:K:100:GLU:O	3:K:102:ARG:N	2.27	0.62
1:A:56:TRP:CE3	1:A:159:GLY:HA3	2.35	0.61
1:A:328:GLY:N	1:A:339:ASN:HD22	1.98	0.61
2:B:62:ARG:O	2:B:66:PRO:HD2	1.99	0.61
2:B:172:LEU:HD12	2:B:172:LEU:H	1.64	0.61
1:E:48:PHE:CB	1:E:394:ASP:HB3	2.29	0.61
1:E:97:ASN:N	1:E:148:GLN:O	2.32	0.61
1:E:139:ARG:NH1	3:G:47:TRP:CZ2	2.68	0.61
1:E:328:GLY:N	1:E:339:ASN:HD22	1.98	0.61
3:G:65:ILE:HG12	5:N:7:UNK:CB	2.30	0.61
1:I:41:GLY:O	1:I:42:GLU:O	2.17	0.61
1:I:72:MET:HG2	1:I:73:VAL:H	1.65	0.61
1:I:145:VAL:HG21	1:I:164:ILE:HD12	1.81	0.61
2:J:34:LEU:HD13	2:J:84:PHE:HE1	1.64	0.61
2:J:166:TRP:CD2	2:J:170:ALA:HB2	2.34	0.61
1:A:108:THR:HB	1:A:134:ASP:HB3	1.81	0.61
1:A:199:HIS:HE1	2:B:128:ALA:N	1.98	0.61
2:B:159:LEU:HG	2:B:247:LYS:NZ	2.14	0.61
2:B:245:THR:C	2:B:247:LYS:H	2.05	0.61
3:C:140:THR:HG22	3:C:141:ASP:H	1.65	0.61
1:E:68:VAL:HG11	1:E:172:ASP:HB2	1.82	0.61
1:E:111:PHE:O	1:E:131:PHE:HB2	1.99	0.61
1:E:361:THR:HG22	1:E:362:ASP:N	2.10	0.61
2:F:38:VAL:CG1	2:F:39:LEU:N	2.62	0.61
2:F:57:VAL:HA	2:F:60:LYS:HG3	1.81	0.61
2:F:98:VAL:O	2:F:101:LEU:N	2.33	0.61
2:F:134:LEU:C	2:F:136:LEU:N	2.58	0.61
2:F:205:VAL:N	2:J:239:VAL:HG11	2.15	0.61
1:I:331:THR:HA	1:I:335:LEU:O	1.99	0.61
1:A:48:PHE:CB	1:A:394:ASP:HB3	2.29	0.61
1:A:95:PHE:O	1:A:150:ASN:N	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:PRO:O	1:A:279:LEU:HB2	1.98	0.61
2:B:98:VAL:O	2:B:101:LEU:N	2.34	0.61
2:B:148:ILE:HG13	2:B:149:THR:N	2.13	0.61
2:B:176:THR:HG22	2:B:177:GLU:N	2.14	0.61
3:C:65:ILE:HG12	5:M:7:UNK:CB	2.30	0.61
5:M:19:UNK:O	5:M:23:UNK:CB	2.48	0.61
1:E:331:THR:HA	1:E:335:LEU:O	1.99	0.61
2:F:166:TRP:CD2	2:F:170:ALA:HB2	2.35	0.61
3:G:44:ILE:HG22	3:G:45:TYR:H	1.66	0.61
1:A:297:ALA:HB3	1:A:416:GLU:O	2.00	0.61
2:B:141:LEU:HB3	2:B:142:LEU:HD12	1.82	0.61
1:E:56:TRP:CE3	1:E:159:GLY:HA3	2.35	0.61
3:G:143:THR:OG1	3:G:146:HIS:HB2	2.01	0.61
1:I:238:ASP:O	1:I:242:VAL:HG23	1.99	0.61
2:J:91:PRO:CG	2:J:141:LEU:HG	2.31	0.61
3:K:44:ILE:HG22	3:K:45:TYR:H	1.66	0.61
1:E:108:THR:HB	1:E:134:ASP:HB3	1.81	0.61
1:E:316:LYS:HE2	1:E:373:THR:HG23	1.81	0.61
2:F:107:ILE:HG22	2:F:108:ASN:N	2.16	0.61
1:I:172:ASP:O	1:I:173:PHE:O	2.17	0.61
1:I:235:ILE:HG22	1:I:236:GLY:N	2.14	0.61
2:J:39:LEU:O	2:J:42:TYR:HB3	2.01	0.61
1:A:226:ILE:HG22	1:A:227:SER:N	2.16	0.61
2:B:39:LEU:HD23	2:B:39:LEU:C	2.24	0.61
2:B:245:THR:CG2	2:B:246:THR:N	2.61	0.61
1:I:56:TRP:CE3	1:I:159:GLY:HA3	2.35	0.61
1:I:179:LEU:HD13	2:J:174:GLN:NE2	2.15	0.61
1:I:225:ARG:HG3	1:I:225:ARG:O	2.01	0.61
3:K:143:THR:OG1	3:K:146:HIS:HB2	2.01	0.61
1:A:107:ARG:HG2	2:B:191:PHE:CD1	2.35	0.61
3:C:110:TRP:HZ3	3:C:163:GLY:HA3	1.66	0.61
3:C:115:ALA:O	3:C:116:VAL:C	2.44	0.61
1:E:52:ARG:HG2	1:E:81:PHE:CE1	2.36	0.61
1:E:74:LEU:O	1:E:132:SER:HA	2.00	0.61
3:G:169:LYS:NZ	3:G:176:ALA:HA	2.16	0.61
2:J:38:VAL:CG1	2:J:39:LEU:N	2.62	0.61
1:A:52:ARG:HG2	1:A:81:PHE:CE1	2.36	0.61
1:A:179:LEU:HD23	1:A:179:LEU:N	2.09	0.61
2:B:39:LEU:O	2:B:42:TYR:HB3	2.01	0.61
2:B:169:ILE:CG2	2:B:170:ALA:N	2.63	0.61
5:M:5:UNK:O	5:M:9:UNK:CB	2.49	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:104:VAL:HA	1:E:139:ARG:HB3	1.82	0.61
2:F:82:ALA:HB3	2:F:231:MET:HG3	1.81	0.61
2:F:169:ILE:CG2	2:F:170:ALA:N	2.63	0.61
5:N:22:UNK:O	5:N:26:UNK:N	2.34	0.61
1:I:52:ARG:HG2	1:I:81:PHE:CE1	2.36	0.61
1:I:95:PHE:O	1:I:150:ASN:N	2.33	0.61
1:I:247:LEU:HB2	2:J:138:ILE:HG21	1.82	0.61
2:J:83:PHE:CE2	4:L:507:UNK:CB	2.83	0.61
3:K:140:THR:HG22	3:K:141:ASP:H	1.65	0.61
1:A:104:VAL:HA	1:A:139:ARG:HB3	1.82	0.61
1:A:238:ASP:O	1:A:242:VAL:HG23	2.00	0.61
2:B:19:ALA:O	2:B:23:VAL:HG21	2.00	0.61
2:B:199:PRO:HD2	3:C:133:HIS:CE1	2.36	0.61
2:B:233:TYR:O	2:B:234:PHE:C	2.43	0.61
1:E:74:LEU:HG	1:E:147:ALA:HB2	1.83	0.61
1:E:247:LEU:HB2	2:F:138:ILE:HG21	1.82	0.61
1:E:265:PHE:CE1	1:E:268:THR:HB	2.35	0.61
2:F:19:ALA:O	2:F:23:VAL:HG21	2.00	0.61
2:F:39:LEU:O	2:F:42:TYR:HB3	2.01	0.61
5:N:5:UNK:O	5:N:9:UNK:CB	2.49	0.61
1:I:328:GLY:N	1:I:339:ASN:HD22	1.98	0.61
2:J:21:GLY:C	2:J:23:VAL:H	2.09	0.61
2:J:48:LEU:CD1	2:J:48:LEU:H	2.14	0.61
3:K:132:TRP:NE1	3:K:143:THR:HB	2.12	0.61
1:A:177:VAL:HG22	1:A:178:THR:N	2.16	0.61
1:A:247:LEU:HB2	2:B:138:ILE:HG21	1.82	0.61
2:B:215:LYS:HE2	4:D:506:UNK:CB	2.31	0.61
5:M:6:UNK:O	5:M:10:UNK:CB	2.49	0.61
1:I:43:LYS:N	1:I:50:ARG:NH2	2.49	0.61
1:I:265:PHE:CE1	1:I:268:THR:HB	2.36	0.61
1:I:297:ALA:HB3	1:I:416:GLU:O	2.00	0.61
2:J:19:ALA:O	2:J:23:VAL:HG21	2.00	0.61
2:J:215:LYS:HE2	4:L:506:UNK:CB	2.31	0.61
1:A:207:ALA:CA	1:A:210:ILE:HD12	2.31	0.60
3:C:78:LEU:O	3:C:81:ALA:HB3	2.01	0.60
2:F:233:TYR:O	2:F:234:PHE:C	2.43	0.60
3:G:125:PHE:CD2	3:G:148:ILE:HB	2.36	0.60
3:G:161:ALA:O	3:G:163:GLY:N	2.35	0.60
2:J:57:VAL:HA	2:J:60:LYS:HG3	1.81	0.60
2:J:169:ILE:CG2	2:J:170:ALA:N	2.63	0.60
5:O:6:UNK:O	5:O:10:UNK:CB	2.49	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:GLU:HA	1:A:45:GLN:HG3	1.82	0.60
1:A:74:LEU:HG	1:A:147:ALA:HB2	1.83	0.60
1:A:212:TYR:O	1:A:212:TYR:HD1	1.83	0.60
2:B:155:LEU:HD13	2:B:159:LEU:HD13	1.83	0.60
2:B:180:GLY:O	1:I:420:PRO:HB2	2.01	0.60
1:E:95:PHE:O	1:E:150:ASN:N	2.33	0.60
2:F:203:ARG:C	2:F:207:ARG:HE	2.08	0.60
1:I:104:VAL:HA	1:I:139:ARG:HB3	1.83	0.60
2:J:98:VAL:O	2:J:101:LEU:N	2.33	0.60
2:J:141:LEU:HB3	2:J:142:LEU:HD12	1.82	0.60
5:O:5:UNK:O	5:O:9:UNK:CB	2.49	0.60
1:A:63:LYS:HB2	1:A:63:LYS:HZ2	1.66	0.60
1:A:106:VAL:HG12	1:A:107:ARG:H	1.65	0.60
1:A:225:ARG:HG3	1:A:225:ARG:O	2.01	0.60
3:C:107:LEU:C	3:C:109:GLU:H	2.09	0.60
1:E:201:PRO:CA	1:E:204:ILE:HD12	2.29	0.60
2:F:235:LEU:O	2:F:236:TRP:C	2.43	0.60
3:K:107:LEU:C	3:K:109:GLU:H	2.09	0.60
3:K:121:GLY:CA	3:K:153:SER:OG	2.50	0.60
1:A:74:LEU:O	1:A:132:SER:HA	2.00	0.60
5:M:22:UNK:O	5:M:26:UNK:N	2.34	0.60
1:E:393:TYR:O	1:I:270:PRO:HG3	2.02	0.60
2:F:54:ASP:OD1	2:F:127:SER:N	2.34	0.60
3:G:121:GLY:CA	3:G:153:SER:OG	2.50	0.60
1:I:178:THR:HG23	1:I:183:THR:O	2.02	0.60
1:I:269:ILE:CD1	2:J:175:ALA:HB2	2.31	0.60
2:J:35:PHE:HB2	2:J:96:PHE:CE2	2.36	0.60
2:J:107:ILE:HG22	2:J:108:ASN:N	2.16	0.60
3:K:124:PHE:C	3:K:126:THR:H	2.10	0.60
1:A:211:LEU:O	1:A:213:TRP:N	2.34	0.60
1:A:299:LEU:HD23	1:A:315:VAL:HG22	1.82	0.60
2:B:235:LEU:O	2:B:236:TRP:C	2.43	0.60
1:E:72:MET:HG2	1:E:73:VAL:H	1.65	0.60
2:F:245:THR:CG2	2:F:246:THR:N	2.61	0.60
3:G:104:HIS:O	3:G:105:VAL:C	2.42	0.60
1:I:106:VAL:HG12	1:I:107:ARG:H	1.66	0.60
1:I:177:VAL:HG22	1:I:178:THR:N	2.16	0.60
1:I:211:LEU:O	1:I:213:TRP:N	2.34	0.60
3:K:169:LYS:NZ	3:K:176:ALA:HA	2.16	0.60
1:A:43:LYS:N	1:A:50:ARG:NH2	2.49	0.60
2:B:166:TRP:HA	2:B:166:TRP:CE3	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:22:ARG:HH11	3:C:22:ARG:CB	2.14	0.60
1:E:207:ALA:CA	1:E:210:ILE:HD12	2.31	0.60
1:E:211:LEU:O	1:E:213:TRP:N	2.34	0.60
2:F:70:PRO:HG3	2:F:161:PHE:CD2	2.37	0.60
1:I:113:GLY:HA3	1:I:279:LEU:CD2	2.25	0.60
2:J:155:LEU:HD13	2:J:159:LEU:HD13	1.83	0.60
5:O:22:UNK:O	5:O:26:UNK:N	2.34	0.60
2:B:35:PHE:HB2	2:B:96:PHE:CE2	2.36	0.60
2:B:182:LEU:HD12	2:B:183:MET:H	1.67	0.60
2:B:206:GLU:OE2	2:B:207:ARG:HG3	2.01	0.60
3:C:144:PRO:O	3:C:147:ILE:HG22	2.02	0.60
1:E:107:ARG:HG2	2:F:191:PHE:HD1	1.67	0.60
1:E:221:ALA:O	1:E:225:ARG:HB2	2.02	0.60
1:E:269:ILE:CD1	2:F:175:ALA:HB2	2.31	0.60
2:F:229:SER:C	2:F:231:MET:N	2.48	0.60
5:N:6:UNK:O	5:N:10:UNK:CB	2.49	0.60
1:I:74:LEU:O	1:I:132:SER:HA	2.00	0.60
3:K:18:ILE:O	3:K:19:VAL:HB	2.01	0.60
3:K:115:ALA:O	3:K:116:VAL:C	2.44	0.60
2:F:155:LEU:HD13	2:F:159:LEU:HD13	1.83	0.60
3:G:56:PRO:C	3:G:58:PHE:H	2.10	0.60
3:G:114:TYR:CE2	3:G:118:ILE:HD11	2.36	0.60
3:G:132:TRP:NE1	3:G:144:PRO:HD2	2.16	0.60
3:G:144:PRO:O	3:G:147:ILE:HG22	2.02	0.60
1:I:359:LEU:HD23	1:I:360:SER:N	2.17	0.60
3:K:161:ALA:O	3:K:163:GLY:N	2.35	0.60
2:B:91:PRO:CG	2:B:141:LEU:HG	2.31	0.60
2:B:237:TRP:C	2:B:237:TRP:CE3	2.80	0.60
3:C:125:PHE:CD2	3:C:148:ILE:HB	2.36	0.60
1:E:212:TYR:HD1	1:E:212:TYR:O	1.83	0.60
1:E:359:LEU:HD23	1:E:360:SER:N	2.17	0.60
2:F:35:PHE:HB2	2:F:96:PHE:CE2	2.36	0.60
2:F:188:LEU:HD22	2:F:192:HIS:CD2	2.37	0.60
1:I:212:TYR:O	1:I:212:TYR:HD1	1.83	0.60
1:I:226:ILE:HG22	1:I:227:SER:N	2.16	0.60
2:J:199:PRO:HD2	3:K:133:HIS:CE1	2.36	0.60
3:K:110:TRP:HZ3	3:K:163:GLY:HA3	1.66	0.60
1:A:270:PRO:HG3	1:I:393:TYR:O	2.02	0.60
2:B:48:LEU:CD1	2:B:48:LEU:H	2.14	0.60
3:C:44:ILE:HG22	3:C:45:TYR:H	1.66	0.60
2:F:91:PRO:CG	2:F:141:LEU:HG	2.30	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:199:PRO:HD2	3:G:133:HIS:CE1	2.36	0.60
2:F:215:LYS:HE2	4:H:506:UNK:CB	2.31	0.60
2:J:206:GLU:OE2	2:J:207:ARG:HG3	2.01	0.60
1:A:221:ALA:O	1:A:225:ARG:HB2	2.02	0.59
2:B:107:ILE:HG22	2:B:108:ASN:N	2.16	0.59
3:C:169:LYS:NZ	3:C:176:ALA:HA	2.16	0.59
1:E:331:THR:HG22	1:E:335:LEU:O	2.02	0.59
2:F:48:LEU:H	2:F:48:LEU:CD1	2.14	0.59
2:F:166:TRP:CE3	2:F:166:TRP:HA	2.36	0.59
3:G:78:LEU:O	3:G:81:ALA:HB3	2.01	0.59
1:I:221:ALA:O	1:I:225:ARG:HB2	2.02	0.59
2:J:166:TRP:HA	2:J:166:TRP:CE3	2.36	0.59
2:J:166:TRP:HB3	2:J:167:PRO:HD3	1.84	0.59
3:K:22:ARG:HH11	3:K:22:ARG:CB	2.14	0.59
3:K:42:GLU:HA	3:K:62:TRP:CZ3	2.37	0.59
3:K:56:PRO:C	3:K:58:PHE:H	2.10	0.59
3:K:114:TYR:CE2	3:K:118:ILE:HD11	2.36	0.59
3:C:121:GLY:CA	3:C:153:SER:OG	2.50	0.59
3:C:143:THR:OG1	3:C:146:HIS:HB2	2.01	0.59
3:C:161:ALA:O	3:C:163:GLY:N	2.34	0.59
1:E:45:GLN:O	1:E:46:GLN:C	2.46	0.59
1:E:106:VAL:HG12	1:E:107:ARG:H	1.66	0.59
1:E:263:SER:C	1:E:265:PHE:N	2.59	0.59
1:E:393:TYR:N	1:E:393:TYR:CD2	2.69	0.59
2:F:237:TRP:C	2:F:237:TRP:CE3	2.80	0.59
3:G:18:ILE:O	3:G:19:VAL:HB	2.01	0.59
2:J:235:LEU:O	2:J:236:TRP:C	2.43	0.59
2:J:247:LYS:HD2	2:J:247:LYS:N	2.17	0.59
3:K:78:LEU:O	3:K:81:ALA:HB3	2.01	0.59
3:K:125:PHE:CD2	3:K:148:ILE:HB	2.36	0.59
1:A:178:THR:HG23	1:A:183:THR:O	2.02	0.59
1:A:180:LEU:C	1:A:182:GLY:H	2.11	0.59
2:B:231:MET:O	2:B:234:PHE:N	2.35	0.59
2:B:238:PHE:HE1	2:B:242:TRP:HB2	1.67	0.59
3:C:42:GLU:HA	3:C:62:TRP:CZ3	2.37	0.59
1:E:177:VAL:HG22	1:E:178:THR:N	2.16	0.59
3:G:83:TRP:O	3:G:87:THR:HG23	2.03	0.59
3:G:110:TRP:HZ3	3:G:163:GLY:HA3	1.66	0.59
2:J:70:PRO:HG3	2:J:161:PHE:CD2	2.37	0.59
2:J:188:LEU:HD22	2:J:192:HIS:CD2	2.37	0.59
2:J:237:TRP:C	2:J:237:TRP:CE3	2.80	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:LEU:HD23	1:A:360:SER:N	2.17	0.59
2:B:70:PRO:HG3	2:B:161:PHE:CD2	2.37	0.59
3:C:114:TYR:CE2	3:C:118:ILE:HD11	2.36	0.59
3:C:132:TRP:NE1	3:C:144:PRO:HD2	2.16	0.59
1:E:299:LEU:HD21	1:E:417:ILE:HG22	1.85	0.59
2:F:182:LEU:HD12	2:F:183:MET:H	1.67	0.59
3:G:115:ALA:O	3:G:116:VAL:C	2.44	0.59
1:I:43:LYS:CA	1:I:50:ARG:HH22	2.16	0.59
2:J:38:VAL:O	2:J:39:LEU:C	2.46	0.59
1:A:72:MET:HG2	1:A:73:VAL:H	1.65	0.59
2:B:54:ASP:OD1	2:B:127:SER:N	2.34	0.59
3:C:102:ARG:HH11	3:C:102:ARG:CG	2.16	0.59
1:E:62:SER:CB	1:E:73:VAL:H	2.13	0.59
1:E:180:LEU:C	1:E:182:GLY:H	2.11	0.59
1:E:297:ALA:HB2	1:E:403:LEU:HD12	1.85	0.59
3:G:107:LEU:C	3:G:109:GLU:H	2.09	0.59
3:K:144:PRO:O	3:K:147:ILE:HG22	2.02	0.59
2:B:83:PHE:CE2	4:D:507:UNK:CB	2.83	0.59
2:B:166:TRP:O	2:B:170:ALA:N	2.36	0.59
1:E:43:LYS:N	1:E:50:ARG:NH2	2.49	0.59
1:E:43:LYS:CA	1:E:50:ARG:HH22	2.16	0.59
1:E:100:GLU:O	1:E:102:GLY:N	2.36	0.59
1:E:178:THR:HG23	1:E:183:THR:O	2.01	0.59
1:E:333:ALA:C	1:E:335:LEU:N	2.59	0.59
2:F:21:GLY:O	2:F:23:VAL:N	2.24	0.59
2:F:21:GLY:C	2:F:23:VAL:H	2.09	0.59
2:F:247:LYS:HD2	2:F:247:LYS:N	2.17	0.59
3:G:106:VAL:O	3:G:109:GLU:HB3	2.03	0.59
1:I:359:LEU:HD23	1:I:360:SER:H	1.68	0.59
2:B:120:PRO:C	2:B:122:SER:N	2.51	0.59
1:E:225:ARG:HG3	1:E:225:ARG:O	2.01	0.59
1:E:226:ILE:HG22	1:E:227:SER:N	2.16	0.59
1:E:390:ASP:C	1:E:392:ALA:H	2.11	0.59
2:F:195:ARG:HB3	3:G:134:MET:HB3	1.85	0.59
2:F:206:GLU:OE2	2:F:207:ARG:HG3	2.01	0.59
2:F:231:MET:O	2:F:234:PHE:N	2.35	0.59
3:G:22:ARG:HH11	3:G:22:ARG:CB	2.15	0.59
3:G:42:GLU:HA	3:G:62:TRP:CZ3	2.37	0.59
1:I:42:GLU:O	1:I:44:SER:N	2.34	0.59
1:I:158:ILE:HG21	3:K:137:ILE:CD1	2.33	0.59
1:I:201:PRO:CA	1:I:204:ILE:HD12	2.29	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:248:ALA:O	1:I:252:LEU:HD23	2.03	0.59
2:J:231:MET:O	2:J:234:PHE:N	2.35	0.59
1:A:138:ARG:HA	1:A:173:PHE:CD1	2.38	0.59
1:A:187:LEU:O	1:A:189:THR:N	2.36	0.59
2:B:195:ARG:HB3	3:C:134:MET:HB3	1.84	0.59
3:C:80:LEU:HD22	3:C:80:LEU:N	2.18	0.59
1:E:226:ILE:HD13	1:E:231:ASP:CB	2.33	0.59
1:I:217:LYS:HD2	2:J:24:LYS:HZ3	1.66	0.59
2:J:108:ASN:HA	2:J:112:ASN:HD22	1.68	0.59
1:A:62:SER:CB	1:A:73:VAL:H	2.13	0.59
1:A:100:GLU:O	1:A:102:GLY:N	2.36	0.59
5:M:20:UNK:O	5:M:24:UNK:CB	2.51	0.59
1:E:207:ALA:HA	1:E:210:ILE:CD1	2.33	0.59
1:I:123:LEU:N	1:I:123:LEU:CD1	2.66	0.59
1:I:187:LEU:O	1:I:189:THR:N	2.36	0.59
3:K:100:GLU:C	3:K:102:ARG:H	2.11	0.59
3:K:102:ARG:HH11	3:K:102:ARG:CG	2.16	0.59
3:K:106:VAL:O	3:K:109:GLU:HB3	2.03	0.59
1:A:217:LYS:HB3	1:A:221:ALA:HB3	1.85	0.59
1:A:269:ILE:CD1	2:B:175:ALA:HB2	2.31	0.59
2:B:200:GLU:CG	2:B:201:TYR:H	2.16	0.59
2:B:247:LYS:HD2	2:B:247:LYS:N	2.17	0.59
3:C:110:TRP:HE3	3:C:164:ALA:HB2	1.68	0.59
1:E:96:LEU:HA	1:E:148:GLN:O	2.03	0.59
1:E:138:ARG:HA	1:E:173:PHE:CD1	2.38	0.59
2:F:108:ASN:HA	2:F:112:ASN:HD22	1.68	0.59
2:F:172:LEU:HD12	2:F:172:LEU:N	2.18	0.59
3:G:24:MET:HG3	3:G:109:GLU:CG	2.33	0.59
3:G:124:PHE:C	3:G:126:THR:H	2.10	0.59
3:G:172:ILE:CG2	3:G:173:PRO:HD2	2.31	0.59
1:I:247:LEU:HB2	2:J:138:ILE:CD1	2.33	0.59
1:I:390:ASP:C	1:I:392:ALA:H	2.11	0.59
1:I:393:TYR:CD2	1:I:393:TYR:N	2.69	0.59
3:K:83:TRP:O	3:K:87:THR:HG23	2.03	0.59
1:A:66:LEU:HD22	1:A:70:GLU:HB3	1.85	0.58
1:A:247:LEU:HB2	2:B:138:ILE:CD1	2.33	0.58
1:A:331:THR:HG22	1:A:335:LEU:O	2.02	0.58
1:A:367:ALA:H	1:A:370:GLU:CD	2.11	0.58
2:B:188:LEU:HD22	2:B:192:HIS:CD2	2.37	0.58
1:E:187:LEU:O	1:E:189:THR:N	2.36	0.58
1:E:359:LEU:HD23	1:E:360:SER:H	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:166:TRP:HA	2:F:166:TRP:HE3	1.68	0.58
1:I:96:LEU:HA	1:I:148:GLN:O	2.03	0.58
2:J:54:ASP:OD1	2:J:127:SER:N	2.34	0.58
2:J:195:ARG:HB3	3:K:134:MET:HB3	1.84	0.58
1:A:248:ALA:O	1:A:252:LEU:HD23	2.03	0.58
2:B:166:TRP:HA	2:B:166:TRP:HE3	1.68	0.58
3:C:56:PRO:C	3:C:58:PHE:H	2.10	0.58
3:C:124:PHE:C	3:C:126:THR:H	2.10	0.58
1:E:217:LYS:HD2	2:F:24:LYS:HZ3	1.68	0.58
3:G:132:TRP:CE2	3:G:144:PRO:HG2	2.39	0.58
1:I:138:ARG:HA	1:I:173:PHE:CD1	2.38	0.58
1:I:207:ALA:CA	1:I:210:ILE:HD12	2.31	0.58
1:I:331:THR:HG22	1:I:335:LEU:O	2.02	0.58
3:K:24:MET:HG3	3:K:109:GLU:CG	2.33	0.58
3:K:35:TYR:OH	3:K:156:ILE:HG21	2.02	0.58
3:K:110:TRP:HE3	3:K:164:ALA:HB2	1.68	0.58
3:C:35:TYR:OH	3:C:156:ILE:HG21	2.02	0.58
3:C:106:VAL:O	3:C:109:GLU:HB3	2.03	0.58
1:E:123:LEU:N	1:E:123:LEU:CD1	2.66	0.58
1:E:248:ALA:O	1:E:252:LEU:HD23	2.03	0.58
2:F:55:PHE:CZ	2:F:113:PHE:HZ	2.21	0.58
2:F:88:PHE:C	2:F:90:LEU:N	2.61	0.58
2:F:124:VAL:O	2:F:125:PHE:HB3	2.03	0.58
1:A:107:ARG:HG2	2:B:191:PHE:HD1	1.67	0.58
1:A:297:ALA:HB2	1:A:403:LEU:HD12	1.85	0.58
1:A:299:LEU:HD21	1:A:417:ILE:HG22	1.85	0.58
2:B:34:LEU:HD13	2:B:84:PHE:HE1	1.64	0.58
2:B:55:PHE:CZ	2:B:113:PHE:HZ	2.21	0.58
3:C:18:ILE:O	3:C:19:VAL:HB	2.01	0.58
3:C:41:TYR:CD2	5:M:6:UNK:CB	2.87	0.58
3:C:83:TRP:O	3:C:87:THR:HG23	2.03	0.58
1:E:247:LEU:HB2	2:F:138:ILE:CD1	2.33	0.58
2:F:203:ARG:CB	2:F:207:ARG:HH21	2.12	0.58
3:G:80:LEU:HD22	3:G:80:LEU:N	2.18	0.58
1:I:66:LEU:HD22	1:I:70:GLU:HB3	1.85	0.58
1:I:74:LEU:HG	1:I:147:ALA:HB2	1.83	0.58
1:A:55:ASN:O	1:A:78:VAL:HG13	2.04	0.58
1:A:359:LEU:HD23	1:A:360:SER:H	1.68	0.58
4:D:508:UNK:O	4:D:509:UNK:C	2.51	0.58
3:G:35:TYR:OH	3:G:156:ILE:HG21	2.02	0.58
5:N:20:UNK:O	5:N:24:UNK:CB	2.51	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:107:ARG:HG2	2:J:191:PHE:HD1	1.67	0.58
1:I:202:TRP:CZ3	1:I:250:THR:HG23	2.39	0.58
1:A:45:GLN:O	1:A:46:GLN:C	2.46	0.58
1:A:158:ILE:HG21	3:C:137:ILE:CD1	2.33	0.58
1:A:207:ALA:HA	1:A:210:ILE:CD1	2.33	0.58
1:A:217:LYS:HB3	1:A:221:ALA:CB	2.34	0.58
2:F:33:LEU:HB2	3:G:112:VAL:HG22	1.85	0.58
2:F:79:ALA:HA	2:F:231:MET:CG	2.33	0.58
3:G:100:GLU:O	3:G:102:ARG:N	2.27	0.58
3:K:132:TRP:NE1	3:K:144:PRO:HD2	2.16	0.58
1:A:123:LEU:N	1:A:123:LEU:CD1	2.66	0.58
1:E:42:GLU:O	1:E:44:SER:N	2.34	0.58
1:E:158:ILE:HG21	3:G:137:ILE:CD1	2.33	0.58
1:I:367:ALA:H	1:I:370:GLU:CD	2.11	0.58
2:J:53:TRP:O	2:J:60:LYS:HD3	2.04	0.58
3:K:132:TRP:CE2	3:K:144:PRO:HG2	2.39	0.58
5:O:20:UNK:O	5:O:24:UNK:CB	2.51	0.58
3:C:88:ARG:HG2	3:C:90:ARG:N	2.08	0.58
1:E:137:ALA:HB1	1:E:166:ILE:HG23	1.86	0.58
1:E:367:ALA:H	1:E:370:GLU:CD	2.11	0.58
2:F:14:HIS:N	3:G:98:ARG:HH12	2.02	0.58
2:F:166:TRP:HB3	2:F:167:PRO:HD3	1.84	0.58
2:F:166:TRP:O	2:F:170:ALA:N	2.36	0.58
2:F:176:THR:HG22	2:F:177:GLU:H	1.69	0.58
4:H:508:UNK:O	4:H:509:UNK:C	2.51	0.58
1:I:55:ASN:O	1:I:78:VAL:HG13	2.04	0.58
2:J:14:HIS:N	3:K:98:ARG:HH12	2.02	0.58
2:J:176:THR:HG22	2:J:177:GLU:H	1.69	0.58
2:J:233:TYR:O	2:J:235:LEU:N	2.37	0.58
1:A:137:ALA:HB1	1:A:166:ILE:HG23	1.86	0.58
1:E:118:PRO:HG2	1:E:119:ARG:HD3	1.85	0.58
1:E:217:LYS:HB3	1:E:221:ALA:CB	2.34	0.58
2:F:83:PHE:CD1	2:F:84:PHE:N	2.72	0.58
3:G:102:ARG:HH11	3:G:102:ARG:CG	2.15	0.58
1:I:217:LYS:HB3	1:I:221:ALA:CB	2.34	0.58
1:I:297:ALA:HB2	1:I:403:LEU:HD12	1.85	0.58
2:J:172:LEU:HD12	2:J:172:LEU:N	2.18	0.58
1:A:42:GLU:O	1:A:44:SER:N	2.34	0.58
1:A:43:LYS:CA	1:A:50:ARG:HH22	2.16	0.58
2:B:166:TRP:HB3	2:B:167:PRO:HD3	1.84	0.58
2:B:240:GLY:HA2	2:B:243:TYR:HB3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:132:TRP:CE2	3:C:144:PRO:HG2	2.39	0.58
5:M:17:UNK:O	5:M:21:UNK:N	2.37	0.58
1:E:271:LEU:HD21	2:F:173:HIS:CE1	2.39	0.58
3:G:41:TYR:CD2	5:N:6:UNK:CB	2.87	0.58
3:G:110:TRP:HE3	3:G:164:ALA:HB2	1.68	0.58
1:I:100:GLU:O	1:I:102:GLY:N	2.36	0.58
1:I:139:ARG:HD2	2:J:118:TYR:CD1	2.39	0.58
1:I:266:PRO:CD	1:I:267:ARG:N	2.67	0.58
1:I:271:LEU:HD21	2:J:173:HIS:CE1	2.39	0.58
2:J:166:TRP:HA	2:J:166:TRP:HE3	1.68	0.58
1:A:113:GLY:HA3	1:A:279:LEU:CD2	2.25	0.57
1:A:139:ARG:HD2	2:B:118:TYR:CD1	2.39	0.57
1:A:336:ARG:HB2	1:A:354:LEU:HB2	1.86	0.57
2:B:53:TRP:O	2:B:60:LYS:HD3	2.04	0.57
2:B:108:ASN:HA	2:B:112:ASN:HD22	1.68	0.57
2:B:172:LEU:HD12	2:B:172:LEU:N	2.18	0.57
1:I:226:ILE:HD13	1:I:231:ASP:CB	2.33	0.57
2:J:90:LEU:O	2:J:92:PHE:N	2.37	0.57
2:J:220:VAL:O	2:J:220:VAL:HG12	2.04	0.57
3:K:41:TYR:CD2	5:O:6:UNK:CB	2.87	0.57
5:O:17:UNK:O	5:O:21:UNK:N	2.37	0.57
1:A:271:LEU:HD21	2:B:173:HIS:CE1	2.39	0.57
1:A:393:TYR:CD1	2:F:249:ILE:HD13	2.39	0.57
2:B:33:LEU:CD1	3:C:111:LEU:HB2	2.34	0.57
2:B:90:LEU:O	2:B:92:PHE:N	2.37	0.57
2:B:210:LEU:O	2:B:212:THR:N	2.37	0.57
2:B:249:ILE:HD13	1:I:393:TYR:CD1	2.39	0.57
1:E:55:ASN:O	1:E:78:VAL:HG13	2.04	0.57
1:E:180:LEU:O	1:E:182:GLY:N	2.38	0.57
1:E:311:LEU:HD11	1:E:399:ILE:HD12	1.86	0.57
1:E:395:THR:HG23	1:I:271:LEU:O	2.04	0.57
1:I:299:LEU:HD21	1:I:417:ILE:HG22	1.85	0.57
2:J:55:PHE:CZ	2:J:113:PHE:HZ	2.21	0.57
2:J:79:ALA:HA	2:J:231:MET:CG	2.33	0.57
2:J:140:MET:SD	2:J:140:MET:C	2.87	0.57
3:K:35:TYR:CZ	3:K:156:ILE:HG21	2.40	0.57
3:K:80:LEU:HD22	3:K:80:LEU:N	2.18	0.57
1:A:226:ILE:HD13	1:A:231:ASP:CB	2.33	0.57
1:A:390:ASP:C	1:A:392:ALA:H	2.11	0.57
2:B:140:MET:SD	2:B:140:MET:C	2.87	0.57
2:B:220:VAL:O	2:B:220:VAL:HG12	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:35:TYR:CZ	3:C:156:ILE:HG21	2.40	0.57
3:C:121:GLY:O	3:C:154:TYR:CE2	2.58	0.57
1:E:66:LEU:HD22	1:E:70:GLU:HB3	1.85	0.57
1:E:173:PHE:CZ	1:E:175:ASP:HB2	2.40	0.57
3:G:100:GLU:C	3:G:102:ARG:H	2.11	0.57
2:J:88:PHE:C	2:J:90:LEU:N	2.61	0.57
3:K:100:GLU:CD	3:K:173:PRO:HG3	2.29	0.57
3:K:172:ILE:HG23	3:K:173:PRO:CD	2.31	0.57
1:A:180:LEU:O	1:A:182:GLY:N	2.38	0.57
1:A:201:PRO:CA	1:A:204:ILE:HD12	2.29	0.57
1:E:336:ARG:HB2	1:E:354:LEU:HB2	1.86	0.57
2:F:33:LEU:CD1	3:G:111:LEU:HB2	2.34	0.57
2:F:210:LEU:O	2:F:212:THR:N	2.37	0.57
1:I:45:GLN:O	1:I:46:GLN:C	2.46	0.57
1:I:118:PRO:HG2	1:I:119:ARG:HD3	1.85	0.57
1:I:311:LEU:HD21	1:I:421:VAL:HG11	1.86	0.57
2:J:33:LEU:CD1	3:K:111:LEU:HB2	2.34	0.57
2:J:33:LEU:HB2	3:K:112:VAL:HG22	1.85	0.57
2:J:240:GLY:HA2	2:J:243:TYR:HB3	1.86	0.57
1:A:96:LEU:HA	1:A:148:GLN:O	2.03	0.57
1:A:103:PRO:O	1:A:138:ARG:NH2	2.38	0.57
3:C:24:MET:HG3	3:C:109:GLU:CG	2.33	0.57
3:C:100:GLU:C	3:C:102:ARG:H	2.11	0.57
1:E:103:PRO:O	1:E:138:ARG:NH2	2.38	0.57
1:E:311:LEU:HD21	1:E:421:VAL:HG11	1.87	0.57
2:F:220:VAL:O	2:F:220:VAL:HG12	2.04	0.57
3:G:34:PHE:C	3:G:34:PHE:CD2	2.83	0.57
3:G:35:TYR:CZ	3:G:156:ILE:HG21	2.40	0.57
1:I:103:PRO:O	1:I:138:ARG:NH2	2.38	0.57
1:I:173:PHE:CZ	1:I:175:ASP:HB2	2.40	0.57
1:I:180:LEU:C	1:I:182:GLY:H	2.11	0.57
2:J:83:PHE:CD1	2:J:84:PHE:N	2.72	0.57
2:J:210:LEU:O	2:J:212:THR:N	2.37	0.57
2:B:14:HIS:N	3:C:98:ARG:HH12	2.02	0.57
2:B:239:VAL:HG11	2:J:205:VAL:N	2.20	0.57
3:C:62:TRP:C	3:C:64:SER:N	2.63	0.57
1:E:381:ALA:HB1	1:E:385:ILE:HD11	1.87	0.57
2:F:140:MET:SD	2:F:140:MET:C	2.87	0.57
1:I:180:LEU:O	1:I:182:GLY:N	2.38	0.57
1:I:336:ARG:HB2	1:I:354:LEU:HB2	1.86	0.57
2:J:33:LEU:HD11	3:K:111:LEU:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:182:LEU:HD12	2:J:183:MET:H	1.67	0.57
3:K:47:TRP:HD1	3:K:51:LEU:HD21	1.70	0.57
1:A:63:LYS:HG3	1:A:64:THR:N	2.14	0.57
1:A:96:LEU:H	1:A:96:LEU:CD2	2.18	0.57
2:B:33:LEU:HB2	3:C:112:VAL:HG22	1.85	0.57
1:E:170:MET:HE3	1:E:188:GLU:OE1	2.05	0.57
2:F:238:PHE:HE1	2:F:242:TRP:HB2	1.67	0.57
2:F:240:GLY:HA2	2:F:243:TYR:HB3	1.86	0.57
3:G:95:VAL:HG12	3:G:96:ALA:N	2.20	0.57
3:G:100:GLU:CD	3:G:173:PRO:HG3	2.30	0.57
2:J:166:TRP:O	2:J:170:ALA:N	2.36	0.57
3:K:114:TYR:HA	3:K:160:MET:SD	2.45	0.57
2:B:83:PHE:CD1	2:B:83:PHE:C	2.83	0.57
2:B:83:PHE:CD1	2:B:84:PHE:N	2.72	0.57
2:B:134:LEU:C	2:B:136:LEU:N	2.58	0.57
1:E:59:VAL:HG11	1:E:160:PRO:HG2	1.87	0.57
1:E:139:ARG:HD2	2:F:118:TYR:CD1	2.39	0.57
1:E:217:LYS:HB3	1:E:221:ALA:HB3	1.85	0.57
1:I:137:ALA:HB1	1:I:166:ILE:HG23	1.86	0.57
1:I:329:GLU:HG3	1:I:338:LEU:CA	2.25	0.57
1:I:352:TYR:O	1:I:382:ARG:HD3	2.05	0.57
4:L:508:UNK:O	4:L:509:UNK:C	2.51	0.57
1:A:59:VAL:HG11	1:A:160:PRO:HG2	1.87	0.57
1:A:352:TYR:O	1:A:382:ARG:HD3	2.05	0.57
3:C:85:TRP:C	3:C:87:THR:N	2.62	0.57
1:E:51:MET:HE1	1:E:388:LEU:HD13	1.87	0.57
1:E:266:PRO:CD	1:E:267:ARG:N	2.67	0.57
2:F:129:LEU:O	2:F:132:PRO:HD2	2.05	0.57
3:G:85:TRP:C	3:G:87:THR:N	2.62	0.57
5:N:17:UNK:O	5:N:21:UNK:N	2.37	0.57
1:A:118:PRO:HG2	1:A:119:ARG:HD3	1.85	0.57
1:A:311:LEU:HD21	1:A:421:VAL:HG11	1.86	0.57
2:B:239:VAL:HG11	2:J:204:MET:C	2.29	0.57
3:C:95:VAL:HG12	3:C:96:ALA:N	2.20	0.57
5:M:1:UNK:N	5:M:4:UNK:CB	2.68	0.57
1:E:146:HIS:HA	1:E:161:GLY:HA3	1.87	0.57
2:F:233:TYR:O	2:F:235:LEU:N	2.37	0.57
1:I:356:ASP:C	1:I:358:GLY:H	2.12	0.57
2:J:238:PHE:HE1	2:J:242:TRP:HB2	1.67	0.57
3:K:95:VAL:HG12	3:K:96:ALA:N	2.20	0.57
1:A:170:MET:HE3	1:A:188:GLU:OE1	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:PHE:CZ	1:A:175:ASP:HB2	2.40	0.56
1:A:233:GLU:CD	1:A:233:GLU:N	2.63	0.56
3:C:47:TRP:HD1	3:C:51:LEU:HD21	1.70	0.56
1:E:96:LEU:H	1:E:96:LEU:CD2	2.18	0.56
1:E:96:LEU:H	1:E:96:LEU:HD23	1.69	0.56
2:F:38:VAL:O	2:F:39:LEU:C	2.46	0.56
2:F:83:PHE:C	2:F:83:PHE:HD1	2.13	0.56
2:F:90:LEU:O	2:F:92:PHE:N	2.37	0.56
2:F:108:ASN:O	2:F:112:ASN:HB2	2.05	0.56
5:N:1:UNK:N	5:N:4:UNK:CB	2.68	0.56
1:I:97:ASN:ND2	2:J:194:VAL:HG11	2.20	0.56
1:I:217:LYS:HB3	1:I:221:ALA:HB3	1.85	0.56
1:I:306:VAL:O	1:I:306:VAL:HG12	2.05	0.56
2:J:83:PHE:CD1	2:J:83:PHE:C	2.83	0.56
2:J:124:VAL:O	2:J:125:PHE:HB3	2.04	0.56
3:K:34:PHE:C	3:K:34:PHE:CD2	2.83	0.56
1:A:329:GLU:HG3	1:A:338:LEU:CA	2.25	0.56
1:A:356:ASP:C	1:A:358:GLY:H	2.12	0.56
1:A:393:TYR:CD2	1:A:393:TYR:N	2.69	0.56
2:B:33:LEU:HD11	3:C:111:LEU:HB2	1.86	0.56
2:B:195:ARG:HB2	3:C:134:MET:HE3	1.87	0.56
2:B:233:TYR:O	2:B:235:LEU:N	2.37	0.56
3:C:100:GLU:O	3:C:102:ARG:N	2.27	0.56
3:C:135:THR:OG1	3:C:136:VAL:N	2.39	0.56
3:C:172:ILE:CG2	3:C:173:PRO:HD2	2.31	0.56
2:F:53:TRP:O	2:F:60:LYS:HD3	2.04	0.56
3:G:121:GLY:O	3:G:154:TYR:CE2	2.58	0.56
1:I:43:LYS:O	1:I:387:ARG:HD3	2.06	0.56
1:I:170:MET:HE3	1:I:188:GLU:OE1	2.05	0.56
1:I:316:LYS:CD	1:I:373:THR:HG23	2.35	0.56
2:J:13:PHE:HZ	2:J:22:CYS:O	1.88	0.56
2:J:83:PHE:C	2:J:83:PHE:HD1	2.13	0.56
1:A:158:ILE:CG2	3:C:137:ILE:HD13	2.36	0.56
1:A:316:LYS:CD	1:A:373:THR:HG23	2.35	0.56
1:A:388:LEU:C	1:A:390:ASP:N	2.61	0.56
2:B:21:GLY:C	2:B:23:VAL:H	2.09	0.56
3:C:100:GLU:CD	3:C:173:PRO:HG3	2.30	0.56
3:C:114:TYR:HA	3:C:160:MET:SD	2.45	0.56
1:E:106:VAL:HG13	2:F:192:HIS:HB3	1.87	0.56
1:E:214:PHE:CZ	2:F:31:LEU:HD22	2.41	0.56
1:E:306:VAL:O	1:E:306:VAL:HG12	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:42:TYR:HA	2:F:76:PHE:CE2	2.40	0.56
2:F:195:ARG:HB2	3:G:134:MET:HE3	1.87	0.56
2:F:235:LEU:C	2:F:235:LEU:CD2	2.79	0.56
2:F:236:TRP:O	2:F:238:PHE:N	2.38	0.56
3:G:119:TYR:CD1	3:G:119:TYR:C	2.84	0.56
1:I:59:VAL:HG11	1:I:160:PRO:HG2	1.87	0.56
1:I:90:ASN:O	1:I:92:LYS:N	2.37	0.56
1:I:94:SER:OG	1:I:151:VAL:HG22	2.05	0.56
1:I:96:LEU:HD23	1:I:96:LEU:H	1.69	0.56
1:I:138:ARG:HD2	1:I:173:PHE:CE2	2.40	0.56
1:I:212:TYR:O	1:I:213:TRP:HE3	1.89	0.56
1:I:311:LEU:HD11	1:I:399:ILE:HD12	1.86	0.56
2:J:81:GLN:OE1	2:J:136:LEU:HD22	2.06	0.56
2:J:200:GLU:CG	2:J:201:TYR:H	2.16	0.56
5:O:1:UNK:N	5:O:4:UNK:CB	2.68	0.56
1:A:90:ASN:O	1:A:92:LYS:N	2.37	0.56
2:B:13:PHE:HZ	2:B:22:CYS:O	1.88	0.56
2:B:42:TYR:HA	2:B:76:PHE:CE2	2.40	0.56
2:B:68:VAL:C	2:B:70:PRO:HD2	2.30	0.56
2:B:108:ASN:O	2:B:112:ASN:HB2	2.05	0.56
2:B:124:VAL:O	2:B:125:PHE:HB3	2.03	0.56
2:B:131:VAL:O	2:B:132:PRO:C	2.49	0.56
1:E:202:TRP:CZ3	1:E:250:THR:HG23	2.39	0.56
1:E:356:ASP:C	1:E:358:GLY:H	2.12	0.56
3:G:114:TYR:HA	3:G:160:MET:SD	2.45	0.56
1:I:253:ALA:HA	1:I:256:ILE:CD1	2.36	0.56
2:J:120:PRO:O	2:J:123:LEU:HD23	2.06	0.56
2:J:195:ARG:HB2	3:K:134:MET:HE3	1.87	0.56
3:K:62:TRP:C	3:K:64:SER:N	2.63	0.56
3:K:121:GLY:O	3:K:154:TYR:CE2	2.58	0.56
1:A:212:TYR:O	1:A:213:TRP:HE3	1.89	0.56
1:A:306:VAL:O	1:A:306:VAL:HG12	2.05	0.56
1:A:391:LEU:HD13	1:A:397:SER:O	2.06	0.56
2:B:38:VAL:O	2:B:39:LEU:C	2.46	0.56
3:C:34:PHE:C	3:C:34:PHE:CD2	2.83	0.56
3:C:69:GLU:OE2	3:C:151:TYR:C	2.49	0.56
1:E:63:LYS:HB2	1:E:63:LYS:HZ2	1.70	0.56
1:E:138:ARG:HD2	1:E:173:PHE:CE2	2.40	0.56
1:E:275:LEU:HD23	1:E:276:GLN:H	1.71	0.56
1:E:311:LEU:HD12	1:E:383:TRP:CZ2	2.41	0.56
2:F:162:TYR:O	2:F:163:PRO:C	2.49	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:47:TRP:HD1	3:G:51:LEU:HD21	1.70	0.56
1:I:51:MET:HE1	1:I:388:LEU:HD13	1.87	0.56
2:J:129:LEU:O	2:J:132:PRO:HD2	2.05	0.56
1:A:138:ARG:HD2	1:A:173:PHE:CE2	2.40	0.56
1:A:146:HIS:HA	1:A:161:GLY:HA3	1.87	0.56
2:B:134:LEU:O	2:B:136:LEU:N	2.39	0.56
2:B:241:LYS:HA	2:B:244:SER:OG	2.06	0.56
1:E:60:LYS:H	1:E:75:SER:HB2	1.71	0.56
1:E:62:SER:HB2	1:E:73:VAL:HG23	1.88	0.56
1:E:67:ASN:O	1:E:137:ALA:HB3	2.06	0.56
2:F:109:ARG:HG2	2:F:109:ARG:NH1	2.19	0.56
1:I:269:ILE:HD11	2:J:175:ALA:HB2	1.88	0.56
1:I:333:ALA:C	1:I:335:LEU:N	2.59	0.56
2:J:162:TYR:O	2:J:163:PRO:C	2.49	0.56
3:K:85:TRP:C	3:K:87:THR:N	2.62	0.56
3:K:119:TYR:CD1	3:K:119:TYR:C	2.84	0.56
1:A:67:ASN:O	1:A:137:ALA:HB3	2.06	0.56
1:A:97:ASN:ND2	2:B:194:VAL:HG11	2.20	0.56
1:A:144:HIS:HA	1:A:163:TRP:HA	1.87	0.56
2:B:81:GLN:OE1	2:B:136:LEU:HD22	2.06	0.56
2:B:160:LEU:O	2:B:161:PHE:C	2.49	0.56
1:E:43:LYS:O	1:E:387:ARG:HD3	2.06	0.56
1:E:144:HIS:HA	1:E:163:TRP:HA	1.87	0.56
1:E:158:ILE:CG2	3:G:137:ILE:HD13	2.36	0.56
1:E:235:ILE:HD11	2:F:89:LYS:HB3	1.88	0.56
2:F:161:PHE:CD1	2:F:161:PHE:C	2.84	0.56
2:F:212:THR:HG22	4:H:502:UNK:CB	2.36	0.56
3:G:69:GLU:OE2	3:G:151:TYR:C	2.49	0.56
1:I:96:LEU:H	1:I:96:LEU:CD2	2.18	0.56
2:J:212:THR:HG22	4:L:502:UNK:CB	2.36	0.56
1:A:106:VAL:HG13	2:B:192:HIS:HB3	1.88	0.56
1:A:235:ILE:HD11	2:B:89:LYS:HB3	1.88	0.56
2:B:203:ARG:CB	2:B:207:ARG:HH21	2.12	0.56
2:B:236:TRP:O	2:B:238:PHE:N	2.38	0.56
1:I:144:HIS:HA	1:I:163:TRP:HA	1.87	0.56
2:J:40:GLY:O	2:J:42:TYR:N	2.39	0.56
1:A:237:ASP:O	1:A:239:ASP:N	2.39	0.56
1:A:253:ALA:HA	1:A:256:ILE:CD1	2.36	0.56
1:A:381:ALA:HB1	1:A:385:ILE:HD11	1.87	0.56
2:B:109:ARG:HG2	2:B:109:ARG:NH1	2.19	0.56
2:B:205:VAL:HG22	2:F:239:VAL:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:37:ILE:O	3:C:40:ILE:N	2.38	0.56
1:E:97:ASN:ND2	2:F:194:VAL:HG11	2.20	0.56
2:F:78:ALA:HB1	2:F:234:PHE:CD1	2.41	0.56
2:F:131:VAL:O	2:F:132:PRO:C	2.49	0.56
2:F:241:LYS:HA	2:F:244:SER:OG	2.06	0.56
1:I:42:GLU:H	1:I:158:ILE:CD1	2.17	0.56
1:I:106:VAL:HG12	2:J:192:HIS:HD1	1.71	0.56
1:I:263:SER:C	1:I:265:PHE:N	2.59	0.56
1:I:381:ALA:HB1	1:I:385:ILE:HD11	1.87	0.56
2:J:42:TYR:HA	2:J:76:PHE:CE2	2.41	0.56
2:J:68:VAL:C	2:J:70:PRO:HD2	2.30	0.56
2:J:108:ASN:O	2:J:112:ASN:HB2	2.05	0.56
1:A:94:SER:OG	1:A:151:VAL:HG22	2.05	0.56
2:B:161:PHE:C	2:B:161:PHE:CD1	2.84	0.56
1:E:42:GLU:H	1:E:158:ILE:CD1	2.17	0.56
1:E:199:HIS:HE1	2:F:127:SER:C	2.13	0.56
2:F:40:GLY:O	2:F:42:TYR:N	2.39	0.56
2:F:83:PHE:CD1	2:F:83:PHE:C	2.83	0.56
2:F:134:LEU:O	2:F:136:LEU:N	2.39	0.56
3:G:24:MET:HG3	3:G:109:GLU:HG2	1.88	0.56
2:J:48:LEU:HD12	2:J:48:LEU:N	2.21	0.56
3:K:24:MET:HG3	3:K:109:GLU:HG2	1.88	0.56
3:K:34:PHE:HE1	5:O:11:UNK:HA	1.70	0.56
3:K:69:GLU:OE2	3:K:151:TYR:C	2.49	0.56
3:K:135:THR:OG1	3:K:136:VAL:N	2.39	0.56
1:A:42:GLU:H	1:A:158:ILE:CD1	2.17	0.55
1:A:48:PHE:C	1:A:48:PHE:HD2	2.14	0.55
1:A:106:VAL:CG1	2:B:192:HIS:HB3	2.37	0.55
1:A:199:HIS:HE1	2:B:127:SER:C	2.13	0.55
2:B:83:PHE:C	2:B:83:PHE:HD1	2.13	0.55
2:B:120:PRO:O	2:B:123:LEU:HD23	2.06	0.55
2:B:146:TYR:CZ	2:B:231:MET:HE1	2.42	0.55
3:C:104:HIS:O	3:C:106:VAL:N	2.39	0.55
1:I:169:ASP:OD2	1:I:171:ALA:HB3	2.06	0.55
2:J:135:TRP:CZ2	2:J:139:ILE:HD11	2.42	0.55
3:K:153:SER:HA	3:K:156:ILE:HB	1.88	0.55
1:A:169:ASP:OD2	1:A:171:ALA:HB3	2.06	0.55
1:A:273:ALA:H	1:I:395:THR:HG22	1.71	0.55
2:B:40:GLY:O	2:B:42:TYR:N	2.39	0.55
2:B:149:THR:HG22	2:B:234:PHE:HZ	1.70	0.55
3:C:111:LEU:HA	3:C:114:TYR:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:352:TYR:O	1:E:382:ARG:HD3	2.05	0.55
1:I:207:ALA:HA	1:I:210:ILE:CD1	2.33	0.55
1:I:299:LEU:O	1:I:301:GLY:N	2.40	0.55
2:J:78:ALA:HB1	2:J:234:PHE:HD1	1.72	0.55
2:J:109:ARG:HG2	2:J:109:ARG:NH1	2.19	0.55
2:J:228:VAL:O	2:J:230:MET:N	2.40	0.55
1:A:214:PHE:CZ	2:B:31:LEU:HD22	2.41	0.55
2:B:164:ASN:OD1	2:B:165:ASN:N	2.40	0.55
3:C:34:PHE:HE1	5:M:11:UNK:HA	1.70	0.55
1:E:48:PHE:C	1:E:48:PHE:HD2	2.14	0.55
1:E:106:VAL:CG1	2:F:192:HIS:HB3	2.37	0.55
1:E:316:LYS:CD	1:E:373:THR:HG23	2.35	0.55
2:F:120:PRO:O	2:F:123:LEU:HD23	2.06	0.55
2:F:149:THR:HG22	2:F:234:PHE:HZ	1.70	0.55
2:F:211:ARG:NH1	3:G:154:TYR:O	2.40	0.55
3:G:153:SER:HA	3:G:156:ILE:HD12	1.88	0.55
1:I:311:LEU:HD12	1:I:383:TRP:CZ2	2.41	0.55
2:J:146:TYR:CZ	2:J:231:MET:HE1	2.42	0.55
2:J:164:ASN:OD1	2:J:165:ASN:N	2.40	0.55
2:J:236:TRP:O	2:J:238:PHE:N	2.38	0.55
2:J:241:LYS:HA	2:J:244:SER:OG	2.06	0.55
3:K:125:PHE:O	3:K:149:GLU:HB2	2.07	0.55
1:A:96:LEU:H	1:A:96:LEU:HD23	1.69	0.55
1:A:237:ASP:HA	1:A:240:ARG:CG	2.37	0.55
1:A:311:LEU:HD11	1:A:399:ILE:HD12	1.86	0.55
2:B:79:ALA:HA	2:B:231:MET:CG	2.33	0.55
2:B:88:PHE:C	2:B:90:LEU:N	2.61	0.55
3:C:153:SER:HA	3:C:156:ILE:HD12	1.88	0.55
3:C:165:PHE:CD2	3:C:166:PHE:N	2.75	0.55
1:E:106:VAL:HG12	2:F:192:HIS:HD1	1.71	0.55
1:E:233:GLU:CD	1:E:233:GLU:N	2.63	0.55
2:F:200:GLU:CG	2:F:201:TYR:H	2.16	0.55
3:G:31:LEU:HD11	3:G:35:TYR:CD1	2.39	0.55
3:G:67:TRP:N	3:G:67:TRP:CD1	2.74	0.55
3:G:135:THR:OG1	3:G:136:VAL:N	2.39	0.55
1:I:214:PHE:CZ	2:J:31:LEU:HD22	2.41	0.55
2:J:78:ALA:HB1	2:J:234:PHE:CD1	2.42	0.55
2:J:146:TYR:O	2:J:147:VAL:C	2.49	0.55
3:K:111:LEU:HA	3:K:114:TYR:HB3	1.88	0.55
1:A:43:LYS:O	1:A:387:ARG:HD3	2.06	0.55
1:A:51:MET:HE1	1:A:388:LEU:HD13	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:SER:HB2	1:A:73:VAL:HG23	1.87	0.55
2:B:50:ALA:C	2:B:52:ASP:H	2.12	0.55
2:B:212:THR:HG22	4:D:502:UNK:CB	2.36	0.55
1:E:196:TYR:O	1:E:200:PHE:HB3	2.06	0.55
1:E:212:TYR:O	1:E:213:TRP:HE3	1.89	0.55
1:E:391:LEU:HD13	1:E:397:SER:O	2.06	0.55
2:F:68:VAL:C	2:F:70:PRO:HD2	2.30	0.55
2:F:71:ILE:O	2:F:73:GLY:N	2.40	0.55
3:G:61:TYR:HA	5:N:3:UNK:CB	2.37	0.55
1:I:60:LYS:H	1:I:75:SER:HB2	1.71	0.55
1:I:124:GLU:OE1	1:I:125:VAL:N	2.37	0.55
1:I:199:HIS:HE1	2:J:127:SER:C	2.13	0.55
1:I:224:LEU:C	1:I:226:ILE:N	2.64	0.55
2:J:134:LEU:O	2:J:136:LEU:N	2.39	0.55
3:K:37:ILE:O	3:K:40:ILE:N	2.38	0.55
1:A:47:ALA:O	1:A:48:PHE:C	2.49	0.55
1:A:78:VAL:HG23	1:A:131:PHE:HE2	1.72	0.55
1:A:299:LEU:O	1:A:301:GLY:N	2.40	0.55
1:A:311:LEU:HD12	1:A:383:TRP:CZ2	2.41	0.55
2:B:51:GLY:O	2:B:52:ASP:HB2	2.06	0.55
2:B:78:ALA:HB1	2:B:234:PHE:HD1	1.72	0.55
2:B:129:LEU:O	2:B:132:PRO:HD2	2.05	0.55
2:B:228:VAL:O	2:B:230:MET:N	2.40	0.55
2:B:231:MET:C	2:B:233:TYR:N	2.60	0.55
3:C:119:TYR:CD1	3:C:119:TYR:C	2.84	0.55
1:E:328:GLY:N	1:E:405:PHE:CE1	2.75	0.55
2:F:146:TYR:CZ	2:F:231:MET:HE1	2.42	0.55
3:G:34:PHE:HE1	5:N:11:UNK:HA	1.70	0.55
3:G:165:PHE:CD2	3:G:166:PHE:N	2.75	0.55
1:I:235:ILE:HD11	2:J:89:LYS:HB3	1.88	0.55
2:J:76:PHE:C	2:J:78:ALA:N	2.65	0.55
2:J:123:LEU:CG	2:J:124:VAL:HG13	2.37	0.55
1:A:202:TRP:CZ3	1:A:250:THR:HG23	2.39	0.55
2:B:71:ILE:O	2:B:73:GLY:N	2.40	0.55
2:B:123:LEU:CG	2:B:124:VAL:HG13	2.37	0.55
2:B:176:THR:HG22	2:B:177:GLU:H	1.69	0.55
1:E:94:SER:OG	1:E:151:VAL:HG22	2.05	0.55
1:E:169:ASP:OD2	1:E:171:ALA:HB3	2.07	0.55
1:E:253:ALA:HA	1:E:256:ILE:CD1	2.36	0.55
3:G:153:SER:HA	3:G:156:ILE:HB	1.88	0.55
1:I:62:SER:HB2	1:I:73:VAL:HG23	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:146:HIS:HA	1:I:161:GLY:HA3	1.87	0.55
1:I:158:ILE:CG2	3:K:137:ILE:HD13	2.36	0.55
1:I:198:TRP:HZ3	2:J:128:ALA:HB2	1.72	0.55
1:I:220:ILE:HG22	1:I:221:ALA:N	2.22	0.55
1:I:391:LEU:HD13	1:I:397:SER:O	2.06	0.55
3:K:165:PHE:CD2	3:K:166:PHE:N	2.75	0.55
1:A:220:ILE:C	1:A:222:SER:H	2.14	0.55
2:B:48:LEU:HD12	2:B:48:LEU:N	2.22	0.55
3:C:67:TRP:CD1	3:C:67:TRP:N	2.74	0.55
1:E:65:SER:HA	1:E:165:GLU:O	2.07	0.55
1:E:269:ILE:HD11	2:F:175:ALA:HB2	1.88	0.55
3:G:34:PHE:O	3:G:38:VAL:HG23	2.07	0.55
3:G:125:PHE:O	3:G:149:GLU:HB2	2.07	0.55
1:I:220:ILE:C	1:I:222:SER:H	2.14	0.55
2:J:45:HIS:O	2:J:47:MET:N	2.40	0.55
1:A:52:ARG:HG2	1:A:81:PHE:HE1	1.72	0.55
1:A:106:VAL:HG12	2:B:192:HIS:HD1	1.71	0.55
1:A:225:ARG:NE	1:A:233:GLU:HB2	2.22	0.55
2:B:78:ALA:HB1	2:B:234:PHE:CD1	2.41	0.55
2:B:205:VAL:CG2	2:F:239:VAL:HG12	2.37	0.55
3:C:66:LEU:C	3:C:66:LEU:HD23	2.32	0.55
1:E:47:ALA:O	1:E:48:PHE:C	2.49	0.55
1:E:90:ASN:O	1:E:92:LYS:N	2.37	0.55
1:E:282:ILE:O	1:E:283:ILE:HG12	2.06	0.55
2:F:13:PHE:HZ	2:F:22:CYS:O	1.88	0.55
2:F:48:LEU:N	2:F:48:LEU:HD12	2.22	0.55
3:G:104:HIS:O	3:G:106:VAL:N	2.39	0.55
1:I:67:ASN:O	1:I:137:ALA:HB3	2.06	0.55
1:I:196:TYR:O	1:I:200:PHE:HB3	2.06	0.55
1:I:388:LEU:C	1:I:390:ASP:N	2.61	0.55
2:J:131:VAL:O	2:J:132:PRO:C	2.49	0.55
2:J:149:THR:HG22	2:J:234:PHE:HZ	1.70	0.55
3:K:153:SER:HA	3:K:156:ILE:HD12	1.88	0.55
1:A:393:TYR:CD1	2:F:249:ILE:HG21	2.42	0.55
2:B:159:LEU:H	2:B:159:LEU:HD12	1.72	0.55
3:C:61:TYR:HA	5:M:3:UNK:CB	2.37	0.55
1:E:100:GLU:OE2	1:E:105:LEU:HB2	2.07	0.55
1:E:148:GLN:HB2	1:E:158:ILE:HG22	1.89	0.55
1:E:173:PHE:HZ	1:E:175:ASP:HB2	1.72	0.55
1:E:299:LEU:O	1:E:301:GLY:N	2.40	0.55
1:E:388:LEU:C	1:E:390:ASP:N	2.61	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:33:LEU:HD11	3:G:111:LEU:HB2	1.86	0.55
2:F:135:TRP:CZ2	2:F:139:ILE:HD11	2.41	0.55
2:F:160:LEU:O	2:F:161:PHE:C	2.49	0.55
1:I:106:VAL:HG11	1:I:175:ASP:OD1	2.07	0.55
2:J:18:GLU:O	2:J:22:CYS:N	2.40	0.55
2:J:52:ASP:CB	2:J:55:PHE:HB2	2.37	0.55
2:J:211:ARG:NH1	3:K:154:TYR:O	2.40	0.55
1:A:148:GLN:HB2	1:A:158:ILE:HG22	1.89	0.54
2:B:45:HIS:O	2:B:47:MET:N	2.40	0.54
3:C:34:PHE:O	3:C:38:VAL:HG23	2.07	0.54
1:E:124:GLU:OE1	1:E:125:VAL:N	2.37	0.54
1:E:196:TYR:N	1:E:196:TYR:CD2	2.76	0.54
1:E:220:ILE:C	1:E:222:SER:H	2.14	0.54
1:E:237:ASP:HA	1:E:240:ARG:CG	2.37	0.54
1:E:261:THR:HG22	2:F:170:ALA:CB	2.37	0.54
2:F:78:ALA:HB1	2:F:234:PHE:HD1	1.71	0.54
2:F:81:GLN:OE1	2:F:136:LEU:HD22	2.06	0.54
2:F:164:ASN:OD1	2:F:165:ASN:N	2.40	0.54
2:F:229:SER:O	2:F:231:MET:N	2.33	0.54
3:G:66:LEU:C	3:G:66:LEU:HD23	2.32	0.54
3:G:89:ASP:O	3:G:91:ASN:N	2.40	0.54
1:I:261:THR:HG22	2:J:170:ALA:CB	2.37	0.54
1:I:303:VAL:HA	1:I:422:ILE:O	2.07	0.54
1:I:307:PRO:CG	1:I:308:GLY:H	2.18	0.54
2:J:114:TRP:HA	2:J:114:TRP:HE3	1.72	0.54
2:J:160:LEU:O	2:J:161:PHE:C	2.49	0.54
3:K:46:GLY:O	3:K:51:LEU:HG	2.07	0.54
1:A:60:LYS:H	1:A:75:SER:HB2	1.71	0.54
1:A:62:SER:HB3	1:A:73:VAL:N	2.16	0.54
1:A:141:GLY:C	1:A:142:ARG:HG3	2.32	0.54
1:A:173:PHE:HZ	1:A:175:ASP:HB2	1.72	0.54
1:A:196:TYR:O	1:A:200:PHE:HB3	2.06	0.54
2:B:18:GLU:O	2:B:22:CYS:N	2.40	0.54
1:E:106:VAL:HG11	1:E:175:ASP:OD1	2.07	0.54
2:F:45:HIS:O	2:F:47:MET:N	2.40	0.54
1:I:237:ASP:O	1:I:239:ASP:N	2.39	0.54
1:I:275:LEU:HD23	1:I:276:GLN:H	1.71	0.54
3:K:29:ALA:O	3:K:31:LEU:N	2.40	0.54
3:K:104:HIS:O	3:K:106:VAL:N	2.39	0.54
1:A:198:TRP:HZ3	2:B:128:ALA:HB2	1.72	0.54
1:A:333:ALA:C	1:A:335:LEU:N	2.59	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:ASP:OD2	1:A:351:ASP:C	2.50	0.54
3:C:153:SER:HA	3:C:156:ILE:HB	1.88	0.54
5:M:22:UNK:O	5:M:26:UNK:CB	2.56	0.54
1:E:103:PRO:HB3	2:F:193:PHE:HA	1.90	0.54
1:E:179:LEU:HD23	1:E:179:LEU:N	2.09	0.54
1:E:225:ARG:NE	1:E:233:GLU:HB2	2.22	0.54
2:F:18:GLU:O	2:F:22:CYS:N	2.40	0.54
2:F:51:GLY:O	2:F:52:ASP:HB2	2.06	0.54
2:F:159:LEU:H	2:F:159:LEU:HD12	1.72	0.54
3:G:29:ALA:O	3:G:31:LEU:N	2.40	0.54
1:I:62:SER:CB	1:I:73:VAL:H	2.13	0.54
1:I:106:VAL:CG1	2:J:192:HIS:HB3	2.37	0.54
1:I:282:ILE:O	1:I:283:ILE:HG12	2.06	0.54
3:K:92:VAL:O	3:K:94:ALA:N	2.41	0.54
1:A:196:TYR:N	1:A:196:TYR:CD2	2.76	0.54
1:A:269:ILE:HD11	2:B:175:ALA:HB2	1.88	0.54
1:A:303:VAL:HA	1:A:422:ILE:O	2.07	0.54
1:A:328:GLY:N	1:A:405:PHE:CE1	2.75	0.54
3:C:31:LEU:HD13	3:C:31:LEU:C	2.33	0.54
3:C:172:ILE:HG23	3:C:173:PRO:CD	2.31	0.54
1:E:237:ASP:O	1:E:239:ASP:N	2.39	0.54
1:E:307:PRO:HG2	1:E:308:GLY:N	2.18	0.54
2:F:48:LEU:H	2:F:48:LEU:HD12	1.73	0.54
2:F:114:TRP:HA	2:F:114:TRP:HE3	1.72	0.54
2:F:123:LEU:CG	2:F:124:VAL:HG13	2.37	0.54
5:N:22:UNK:O	5:N:26:UNK:CB	2.56	0.54
1:I:148:GLN:HB2	1:I:158:ILE:HG22	1.89	0.54
1:I:150:ASN:HD21	1:I:156:PRO:CB	2.21	0.54
1:I:328:GLY:N	1:I:405:PHE:CE1	2.75	0.54
3:K:22:ARG:C	3:K:24:MET:H	2.15	0.54
5:O:22:UNK:O	5:O:26:UNK:CB	2.56	0.54
1:A:224:LEU:C	1:A:226:ILE:N	2.64	0.54
2:B:35:PHE:HB2	2:B:96:PHE:HE2	1.72	0.54
2:B:211:ARG:NH1	3:C:154:TYR:O	2.40	0.54
3:C:89:ASP:O	3:C:91:ASN:N	2.40	0.54
1:E:150:ASN:HD21	1:E:156:PRO:CB	2.21	0.54
1:E:307:PRO:CG	1:E:308:GLY:H	2.18	0.54
3:G:92:VAL:O	3:G:94:ALA:N	2.41	0.54
1:I:63:LYS:HE2	1:I:66:LEU:HD23	1.90	0.54
2:J:71:ILE:O	2:J:73:GLY:N	2.40	0.54
3:K:61:TYR:HA	5:O:3:UNK:CB	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:67:TRP:N	3:K:67:TRP:CD1	2.74	0.54
3:K:89:ASP:O	3:K:91:ASN:N	2.40	0.54
1:A:103:PRO:HB3	2:B:193:PHE:HA	1.90	0.54
1:A:220:ILE:HG22	1:A:221:ALA:N	2.22	0.54
2:B:76:PHE:C	2:B:78:ALA:N	2.65	0.54
2:B:82:ALA:CB	2:B:146:TYR:OH	2.55	0.54
2:B:114:TRP:HA	2:B:114:TRP:HE3	1.72	0.54
2:B:146:TYR:O	2:B:147:VAL:C	2.49	0.54
3:C:46:GLY:O	3:C:51:LEU:HG	2.06	0.54
1:E:78:VAL:HG23	1:E:131:PHE:HE2	1.72	0.54
1:E:303:VAL:HA	1:E:422:ILE:O	2.07	0.54
1:E:351:ASP:C	1:E:351:ASP:OD2	2.50	0.54
2:F:52:ASP:CB	2:F:55:PHE:HB2	2.37	0.54
2:F:82:ALA:O	2:F:86:GLU:HB2	2.08	0.54
2:F:119:PHE:HB3	2:F:123:LEU:CD2	2.38	0.54
2:F:196:THR:O	3:G:134:MET:HE1	2.08	0.54
3:G:37:ILE:O	3:G:40:ILE:N	2.38	0.54
3:G:111:LEU:HA	3:G:114:TYR:HB3	1.88	0.54
1:I:52:ARG:HG2	1:I:81:PHE:HE1	1.72	0.54
1:I:107:ARG:NH2	2:J:191:PHE:CD1	2.70	0.54
2:J:48:LEU:H	2:J:48:LEU:HD12	1.73	0.54
2:J:229:SER:O	2:J:231:MET:N	2.33	0.54
1:A:100:GLU:OE2	1:A:105:LEU:HB2	2.07	0.54
1:A:150:ASN:HD21	1:A:156:PRO:CB	2.21	0.54
1:A:188:GLU:HG2	2:B:193:PHE:HE2	1.73	0.54
1:A:273:ALA:H	1:I:395:THR:CG2	2.21	0.54
2:B:135:TRP:CZ2	2:B:139:ILE:HD11	2.42	0.54
2:B:146:TYR:CE2	2:B:231:MET:HE1	2.43	0.54
3:C:92:VAL:O	3:C:94:ALA:N	2.41	0.54
1:E:107:ARG:NH2	2:F:191:PHE:HD1	2.03	0.54
1:E:202:TRP:HB3	2:F:130:VAL:HG11	1.90	0.54
2:F:76:PHE:C	2:F:78:ALA:N	2.65	0.54
2:F:146:TYR:CE2	2:F:231:MET:HE1	2.43	0.54
2:J:114:TRP:CE2	2:J:121:ILE:HD11	2.43	0.54
1:A:63:LYS:HE2	1:A:66:LEU:HD23	1.89	0.54
1:A:275:LEU:HD23	1:A:276:GLN:H	1.71	0.54
2:B:82:ALA:O	2:B:86:GLU:HB2	2.08	0.54
2:B:83:PHE:HD1	2:B:84:PHE:N	2.05	0.54
3:C:29:ALA:O	3:C:31:LEU:N	2.40	0.54
1:E:190:TYR:CD2	1:E:191:GLY:N	2.76	0.54
1:E:223:TYR:CD1	1:E:223:TYR:C	2.85	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:361:THR:CG2	1:E:362:ASP:H	2.16	0.54
3:G:46:GLY:O	3:G:51:LEU:HG	2.06	0.54
1:I:47:ALA:O	1:I:48:PHE:C	2.50	0.54
1:I:106:VAL:HG13	2:J:192:HIS:HB3	1.88	0.54
2:J:161:PHE:C	2:J:161:PHE:CD1	2.84	0.54
3:K:27:GLY:O	3:K:28:VAL:C	2.51	0.54
1:A:65:SER:HA	1:A:165:GLU:O	2.07	0.54
1:A:106:VAL:HG11	1:A:175:ASP:OD1	2.07	0.54
2:B:48:LEU:H	2:B:48:LEU:HD12	1.73	0.54
3:C:125:PHE:O	3:C:149:GLU:HB2	2.07	0.54
1:E:220:ILE:HG22	1:E:221:ALA:N	2.22	0.54
1:E:277:LYS:N	1:E:278:PRO:CD	2.71	0.54
2:F:35:PHE:HB2	2:F:96:PHE:HE2	1.72	0.54
1:A:48:PHE:HB2	1:A:394:ASP:HB3	1.90	0.54
1:A:190:TYR:CD2	1:A:191:GLY:N	2.76	0.54
1:A:223:TYR:CD1	1:A:223:TYR:C	2.85	0.54
1:A:261:THR:HG22	2:B:170:ALA:CB	2.37	0.54
2:B:207:ARG:C	2:B:209:THR:H	2.16	0.54
3:C:67:TRP:CD1	3:C:67:TRP:H	2.26	0.54
1:E:48:PHE:HB2	1:E:394:ASP:HB3	1.90	0.54
1:E:114:GLU:HG3	1:E:280:THR:CB	2.18	0.54
1:E:364:THR:HG22	1:E:372:LYS:HZ3	1.73	0.54
1:E:401:GLY:O	1:E:417:ILE:HG12	2.08	0.54
1:I:190:TYR:CD2	1:I:191:GLY:N	2.76	0.54
1:I:225:ARG:NE	1:I:233:GLU:HB2	2.22	0.54
1:I:277:LYS:N	1:I:278:PRO:CD	2.71	0.54
1:I:374:ILE:HD12	1:I:375:GLU:N	2.23	0.54
2:J:196:THR:O	3:K:134:MET:HE1	2.08	0.54
3:K:66:LEU:C	3:K:66:LEU:HD23	2.32	0.54
5:O:3:UNK:O	5:O:7:UNK:N	2.41	0.54
2:B:39:LEU:HD12	2:B:100:GLY:HA2	1.90	0.53
2:B:114:TRP:HA	2:B:114:TRP:CE3	2.43	0.53
2:F:114:TRP:CE2	2:F:121:ILE:HD11	2.43	0.53
3:G:31:LEU:C	3:G:31:LEU:HD13	2.33	0.53
3:G:137:ILE:O	3:G:138:ARG:O	2.26	0.53
3:G:147:ILE:HD13	3:G:147:ILE:O	2.08	0.53
3:G:172:ILE:HG23	3:G:173:PRO:CD	2.31	0.53
1:I:100:GLU:OE2	1:I:105:LEU:HB2	2.07	0.53
1:I:103:PRO:HB3	2:J:193:PHE:HA	1.90	0.53
1:I:110:GLN:HA	1:I:133:ILE:HG22	1.90	0.53
1:I:141:GLY:C	1:I:142:ARG:HG3	2.32	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:132:PRO:O	2:J:133:ALA:C	2.51	0.53
1:A:51:MET:SD	1:A:399:ILE:CG1	2.96	0.53
2:B:139:ILE:O	2:B:139:ILE:HG22	2.08	0.53
3:C:24:MET:HG3	3:C:109:GLU:HG2	1.88	0.53
1:E:141:GLY:C	1:E:142:ARG:HG3	2.31	0.53
1:E:295:VAL:N	1:E:413:TYR:CD2	2.76	0.53
2:F:238:PHE:CD1	2:F:238:PHE:C	2.87	0.53
1:I:271:LEU:HD11	2:J:60:LYS:O	2.08	0.53
2:J:83:PHE:HD1	2:J:84:PHE:N	2.05	0.53
2:J:227:PHE:C	2:J:229:SER:H	2.16	0.53
3:K:88:ARG:HG2	3:K:90:ARG:N	2.08	0.53
1:A:271:LEU:HD11	2:B:60:LYS:O	2.08	0.53
1:A:421:VAL:C	1:A:422:ILE:HD12	2.34	0.53
2:B:114:TRP:CE2	2:B:121:ILE:HD11	2.43	0.53
2:B:196:THR:O	3:C:134:MET:HE1	2.08	0.53
1:E:63:LYS:HE2	1:E:66:LEU:HD23	1.90	0.53
2:F:39:LEU:HD12	2:F:100:GLY:HA2	1.90	0.53
2:F:114:TRP:HA	2:F:114:TRP:CE3	2.43	0.53
3:G:27:GLY:O	3:G:28:VAL:C	2.51	0.53
2:J:51:GLY:O	2:J:52:ASP:HB2	2.06	0.53
1:A:179:LEU:O	1:A:180:LEU:C	2.52	0.53
3:C:27:GLY:O	3:C:28:VAL:C	2.51	0.53
3:C:137:ILE:O	3:C:138:ARG:O	2.26	0.53
3:C:147:ILE:O	3:C:147:ILE:HD13	2.08	0.53
1:E:79:HIS:CD2	1:E:80:VAL:N	2.77	0.53
2:F:82:ALA:CB	2:F:146:TYR:OH	2.55	0.53
2:F:83:PHE:HD1	2:F:84:PHE:N	2.05	0.53
5:N:3:UNK:O	5:N:7:UNK:N	2.41	0.53
1:I:92:LYS:O	1:I:122:SER:HA	2.09	0.53
1:I:202:TRP:HB3	2:J:130:VAL:HG11	1.90	0.53
1:I:421:VAL:C	1:I:422:ILE:HD12	2.34	0.53
2:B:43:HIS:O	2:B:44:ILE:C	2.52	0.53
2:B:52:ASP:CB	2:B:55:PHE:HB2	2.37	0.53
3:C:41:TYR:CZ	3:C:65:ILE:HD11	2.43	0.53
1:E:198:TRP:HZ3	2:F:128:ALA:HB2	1.72	0.53
1:E:271:LEU:HD11	2:F:60:LYS:O	2.08	0.53
2:F:132:PRO:O	2:F:133:ALA:C	2.51	0.53
2:F:146:TYR:O	2:F:147:VAL:C	2.49	0.53
2:F:207:ARG:C	2:F:209:THR:H	2.16	0.53
2:F:228:VAL:O	2:F:230:MET:N	2.40	0.53
3:G:80:LEU:H	3:G:80:LEU:CD2	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:47:ALA:O	1:I:50:ARG:N	2.42	0.53
2:J:43:HIS:O	2:J:44:ILE:C	2.52	0.53
2:J:238:PHE:CD1	2:J:241:LYS:HB2	2.41	0.53
3:K:163:GLY:C	3:K:165:PHE:H	2.17	0.53
1:A:220:ILE:C	1:A:222:SER:N	2.65	0.53
2:B:55:PHE:HB3	2:B:56:TRP:CD1	2.44	0.53
2:B:206:GLU:CD	2:B:206:GLU:N	2.67	0.53
2:B:235:LEU:HD23	2:B:236:TRP:N	2.24	0.53
3:C:36:LEU:O	3:C:39:ARG:HB3	2.09	0.53
3:C:132:TRP:NE1	3:C:144:PRO:HG2	2.24	0.53
3:C:161:ALA:C	3:C:163:GLY:H	2.17	0.53
5:M:3:UNK:O	5:M:7:UNK:N	2.41	0.53
1:E:92:LYS:O	1:E:122:SER:HA	2.09	0.53
1:E:188:GLU:HG2	2:F:193:PHE:HE2	1.73	0.53
2:F:150:ALA:HA	2:F:234:PHE:HE2	1.73	0.53
2:F:240:GLY:C	2:F:243:TYR:H	2.17	0.53
1:I:220:ILE:C	1:I:222:SER:N	2.65	0.53
2:J:35:PHE:HB2	2:J:96:PHE:HE2	1.72	0.53
2:J:114:TRP:HA	2:J:114:TRP:CE3	2.43	0.53
2:B:107:ILE:HG21	3:C:119:TYR:OH	2.09	0.53
2:B:150:ALA:HA	2:B:234:PHE:HE2	1.73	0.53
1:E:110:GLN:HA	1:E:133:ILE:HG22	1.90	0.53
3:G:36:LEU:O	3:G:39:ARG:HB3	2.09	0.53
1:I:63:LYS:HB3	1:I:66:LEU:HG	1.91	0.53
1:I:65:SER:HA	1:I:165:GLU:O	2.07	0.53
1:I:78:VAL:HG23	1:I:131:PHE:HE2	1.72	0.53
1:I:188:GLU:HG2	2:J:193:PHE:HE2	1.73	0.53
1:I:295:VAL:N	1:I:413:TYR:CD2	2.76	0.53
2:J:82:ALA:O	2:J:86:GLU:HB2	2.08	0.53
3:K:34:PHE:O	3:K:38:VAL:HG23	2.07	0.53
3:K:137:ILE:O	3:K:138:ARG:O	2.26	0.53
3:K:172:ILE:CG2	3:K:173:PRO:HD2	2.31	0.53
1:A:267:ARG:CZ	1:I:425:PHE:HB2	2.39	0.53
1:A:295:VAL:N	1:A:413:TYR:CD2	2.76	0.53
2:B:119:PHE:HB3	2:B:123:LEU:CD2	2.38	0.53
2:B:151:VAL:HG22	2:B:237:TRP:NE1	2.24	0.53
1:E:54:LEU:HD21	1:E:80:VAL:HG13	1.91	0.53
2:F:13:PHE:CD1	2:F:19:ALA:HA	2.44	0.53
1:I:233:GLU:CD	1:I:233:GLU:N	2.63	0.53
1:I:351:ASP:OD2	1:I:351:ASP:C	2.50	0.53
2:J:159:LEU:H	2:J:159:LEU:HD12	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:203:ARG:HA	3:K:150:PHE:HZ	1.74	0.53
2:J:207:ARG:C	2:J:209:THR:H	2.16	0.53
3:K:31:LEU:HD13	3:K:31:LEU:C	2.33	0.53
3:K:34:PHE:HD2	3:K:35:TYR:N	2.07	0.53
1:A:94:SER:O	1:A:120:SER:HA	2.09	0.53
1:A:107:ARG:NH2	2:B:191:PHE:HD1	2.03	0.53
1:A:282:ILE:O	1:A:283:ILE:HG12	2.06	0.53
2:B:33:LEU:C	2:B:33:LEU:CD2	2.82	0.53
2:B:156:GLY:HA2	2:B:159:LEU:HD13	1.91	0.53
2:B:203:ARG:HA	3:C:150:PHE:HZ	1.73	0.53
2:B:239:VAL:CG1	2:J:205:VAL:CA	2.87	0.53
3:C:34:PHE:HD2	3:C:35:TYR:N	2.07	0.53
3:C:89:ASP:CB	3:C:92:VAL:HG22	2.26	0.53
3:C:165:PHE:CD2	3:C:165:PHE:C	2.87	0.53
2:F:107:ILE:HG21	3:G:119:TYR:OH	2.09	0.53
2:F:238:PHE:CG	2:F:239:VAL:N	2.77	0.53
3:G:41:TYR:CZ	3:G:65:ILE:HD11	2.43	0.53
3:G:126:THR:HA	3:G:149:GLU:OE2	2.09	0.53
3:G:132:TRP:NE1	3:G:144:PRO:HG2	2.24	0.53
1:I:198:TRP:C	1:I:200:PHE:H	2.17	0.53
1:I:207:ALA:HA	1:I:210:ILE:HB	1.91	0.53
1:I:219:ILE:O	1:I:220:ILE:HB	2.09	0.53
2:J:85:TRP:CD1	2:J:85:TRP:C	2.87	0.53
2:J:206:GLU:CD	2:J:206:GLU:N	2.67	0.53
5:O:1:UNK:H	5:O:4:UNK:CB	2.22	0.53
1:A:47:ALA:O	1:A:50:ARG:N	2.42	0.53
1:A:110:GLN:HA	1:A:133:ILE:HG22	1.90	0.53
3:C:163:GLY:C	3:C:165:PHE:H	2.17	0.53
2:F:90:LEU:CD1	2:F:92:PHE:HB3	2.39	0.53
2:F:154:SER:O	2:F:157:TRP:HB3	2.09	0.53
2:F:203:ARG:HA	3:G:150:PHE:HZ	1.74	0.53
2:F:231:MET:C	2:F:233:TYR:N	2.60	0.53
2:F:235:LEU:HD23	2:F:236:TRP:N	2.24	0.53
3:G:114:TYR:N	3:G:160:MET:HE1	2.24	0.53
3:G:165:PHE:CD2	3:G:165:PHE:C	2.87	0.53
1:I:401:GLY:O	1:I:417:ILE:HG12	2.08	0.53
2:J:146:TYR:CE2	2:J:231:MET:HE1	2.43	0.53
3:K:170:THR:O	3:K:171:ARG:HG3	2.09	0.53
1:A:84:TRP:CH2	1:A:91:PRO:HB3	2.45	0.52
2:B:162:TYR:O	2:B:163:PRO:C	2.49	0.52
1:E:63:LYS:HG3	1:E:64:THR:N	2.14	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:206:GLU:CD	2:F:206:GLU:N	2.67	0.52
3:G:161:ALA:C	3:G:163:GLY:H	2.17	0.52
1:I:48:PHE:HB2	1:I:394:ASP:HB3	1.90	0.52
1:I:144:HIS:HD1	1:I:163:TRP:NE1	2.07	0.52
1:I:276:GLN:OE1	1:I:276:GLN:N	2.42	0.52
2:J:240:GLY:C	2:J:243:TYR:H	2.17	0.52
3:K:41:TYR:CZ	3:K:65:ILE:HD11	2.43	0.52
3:K:80:LEU:HD23	3:K:159:ILE:HG22	1.91	0.52
3:K:89:ASP:HB3	3:K:92:VAL:CG2	2.25	0.52
1:A:276:GLN:C	1:A:278:PRO:CD	2.81	0.52
1:A:276:GLN:OE1	1:A:276:GLN:N	2.42	0.52
2:B:132:PRO:O	2:B:133:ALA:C	2.51	0.52
3:C:126:THR:HA	3:C:149:GLU:OE2	2.09	0.52
3:C:170:THR:O	3:C:171:ARG:HG3	2.09	0.52
1:E:198:TRP:C	1:E:200:PHE:H	2.17	0.52
2:F:55:PHE:HB3	2:F:56:TRP:CD1	2.44	0.52
2:F:200:GLU:HB3	3:G:138:ARG:HH11	1.74	0.52
3:G:34:PHE:HD2	3:G:35:TYR:N	2.07	0.52
3:G:163:GLY:C	3:G:165:PHE:H	2.17	0.52
2:J:154:SER:O	2:J:157:TRP:HB3	2.09	0.52
2:J:200:GLU:HB3	3:K:138:ARG:HH11	1.74	0.52
2:J:231:MET:C	2:J:233:TYR:N	2.60	0.52
3:K:147:ILE:O	3:K:147:ILE:HD13	2.08	0.52
1:A:79:HIS:CD2	1:A:80:VAL:N	2.77	0.52
1:A:219:ILE:O	1:A:220:ILE:HB	2.09	0.52
1:A:277:LYS:N	1:A:278:PRO:CD	2.71	0.52
2:B:148:ILE:HG13	2:B:149:THR:H	1.75	0.52
1:E:51:MET:SD	1:E:399:ILE:CG1	2.96	0.52
1:E:84:TRP:CH2	1:E:91:PRO:HB3	2.45	0.52
1:E:374:ILE:HD12	1:E:375:GLU:N	2.23	0.52
1:E:421:VAL:C	1:E:422:ILE:HD12	2.34	0.52
2:F:139:ILE:HG22	2:F:139:ILE:O	2.08	0.52
2:F:151:VAL:HG22	2:F:237:TRP:NE1	2.24	0.52
3:G:22:ARG:C	3:G:24:MET:H	2.15	0.52
3:G:96:ALA:O	3:G:99:GLU:N	2.43	0.52
1:I:51:MET:SD	1:I:399:ILE:CG1	2.96	0.52
1:I:54:LEU:HD21	1:I:80:VAL:HG13	1.91	0.52
1:I:84:TRP:CH2	1:I:91:PRO:HB3	2.44	0.52
1:I:94:SER:O	1:I:120:SER:HA	2.09	0.52
1:I:107:ARG:NH2	2:J:191:PHE:HD1	2.03	0.52
1:I:200:PHE:C	1:I:202:TRP:H	2.17	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:364:THR:HG22	1:I:372:LYS:HZ3	1.74	0.52
1:I:371:THR:O	1:I:372:LYS:HG3	2.10	0.52
1:I:393:TYR:O	1:I:394:ASP:C	2.52	0.52
2:J:50:ALA:C	2:J:52:ASP:H	2.12	0.52
2:J:55:PHE:HB3	2:J:56:TRP:CD1	2.44	0.52
2:J:156:GLY:HA2	2:J:159:LEU:HD13	1.91	0.52
2:J:204:MET:C	2:J:206:GLU:OE2	2.53	0.52
3:K:80:LEU:H	3:K:80:LEU:CD2	2.22	0.52
3:K:102:ARG:CG	3:K:102:ARG:NH1	2.73	0.52
3:K:114:TYR:N	3:K:160:MET:HE1	2.24	0.52
1:A:374:ILE:HD12	1:A:375:GLU:N	2.23	0.52
2:B:238:PHE:CD1	2:B:238:PHE:C	2.87	0.52
3:C:22:ARG:C	3:C:24:MET:N	2.66	0.52
1:E:47:ALA:O	1:E:50:ARG:N	2.42	0.52
1:E:179:LEU:O	1:E:180:LEU:C	2.52	0.52
2:F:50:ALA:C	2:F:52:ASP:H	2.12	0.52
2:F:68:VAL:O	2:F:69:VAL:C	2.53	0.52
5:N:1:UNK:H	5:N:4:UNK:CB	2.22	0.52
1:I:44:SER:O	1:I:45:GLN:HG2	2.09	0.52
1:I:202:TRP:HB3	2:J:130:VAL:CB	2.40	0.52
1:I:223:TYR:CD1	1:I:223:TYR:C	2.85	0.52
1:I:237:ASP:HA	1:I:240:ARG:CG	2.37	0.52
2:J:39:LEU:HD12	2:J:100:GLY:HA2	1.90	0.52
2:J:210:LEU:HD23	3:K:158:SER:OG	2.10	0.52
3:K:126:THR:HA	3:K:149:GLU:OE2	2.09	0.52
1:A:213:TRP:HA	1:A:213:TRP:CE3	2.45	0.52
1:A:242:VAL:O	1:A:246:VAL:HG23	2.10	0.52
2:B:21:GLY:C	2:B:23:VAL:N	2.68	0.52
2:B:229:SER:O	2:B:231:MET:N	2.33	0.52
2:B:238:PHE:CG	2:B:239:VAL:N	2.77	0.52
3:C:24:MET:CG	3:C:109:GLU:HG2	2.40	0.52
1:E:276:GLN:OE1	1:E:276:GLN:N	2.42	0.52
1:E:393:TYR:O	1:E:394:ASP:C	2.52	0.52
2:F:43:HIS:O	2:F:44:ILE:C	2.52	0.52
2:F:90:LEU:HD13	2:F:92:PHE:HB3	1.91	0.52
2:F:210:LEU:HD23	3:G:158:SER:OG	2.10	0.52
3:G:118:ILE:O	3:G:121:GLY:N	2.43	0.52
1:I:276:GLN:C	1:I:278:PRO:CD	2.81	0.52
2:J:33:LEU:C	2:J:33:LEU:CD2	2.82	0.52
2:J:174:GLN:NE2	2:J:185:LEU:HD11	2.25	0.52
2:J:186:ALA:O	2:J:187:ASP:C	2.53	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:SER:O	1:A:45:GLN:HG2	2.09	0.52
1:A:173:PHE:O	1:A:174:LYS:HG2	2.10	0.52
1:A:202:TRP:HB3	2:B:130:VAL:CB	2.40	0.52
1:A:364:THR:HG22	1:A:372:LYS:HZ3	1.74	0.52
1:A:401:GLY:O	1:A:417:ILE:HG12	2.08	0.52
2:B:90:LEU:CD1	2:B:92:PHE:HB3	2.39	0.52
2:B:186:ALA:O	2:B:187:ASP:C	2.53	0.52
3:C:118:ILE:O	3:C:121:GLY:N	2.42	0.52
4:D:509:UNK:O	4:D:513:UNK:CB	2.58	0.52
5:M:3:UNK:O	5:M:7:UNK:CB	2.58	0.52
1:E:94:SER:O	1:E:120:SER:HA	2.09	0.52
1:E:200:PHE:C	1:E:202:TRP:H	2.17	0.52
1:E:207:ALA:HA	1:E:210:ILE:HB	1.91	0.52
2:F:204:MET:C	2:F:206:GLU:OE2	2.53	0.52
3:G:56:PRO:C	3:G:58:PHE:N	2.68	0.52
3:G:80:LEU:HD23	3:G:159:ILE:HG22	1.91	0.52
1:I:180:LEU:C	1:I:182:GLY:N	2.66	0.52
2:J:13:PHE:CD1	2:J:19:ALA:HA	2.44	0.52
2:J:90:LEU:CD1	2:J:92:PHE:HB3	2.39	0.52
2:J:139:ILE:O	2:J:139:ILE:HG22	2.08	0.52
3:K:56:PRO:C	3:K:58:PHE:N	2.68	0.52
3:K:67:TRP:CD1	3:K:67:TRP:H	2.26	0.52
3:K:85:TRP:O	3:K:87:THR:N	2.42	0.52
1:A:202:TRP:HB3	2:B:130:VAL:HG11	1.90	0.52
2:B:200:GLU:HB3	3:C:138:ARG:HH11	1.74	0.52
2:B:238:PHE:CD1	2:B:241:LYS:HB2	2.41	0.52
1:E:242:VAL:O	1:E:246:VAL:HG23	2.10	0.52
3:G:170:THR:O	3:G:171:ARG:HG3	2.09	0.52
2:J:238:PHE:CD1	2:J:238:PHE:C	2.87	0.52
3:K:36:LEU:O	3:K:39:ARG:HB3	2.09	0.52
3:K:165:PHE:CD2	3:K:165:PHE:C	2.87	0.52
1:A:105:LEU:CD2	1:A:135:LEU:HD13	2.37	0.52
2:B:38:VAL:HG13	2:B:39:LEU:N	2.25	0.52
2:B:85:TRP:CD1	2:B:85:TRP:C	2.87	0.52
1:E:40:HIS:N	1:E:40:HIS:ND1	2.57	0.52
1:E:180:LEU:C	1:E:182:GLY:N	2.66	0.52
1:E:192:ILE:CD1	2:F:121:ILE:HD13	2.31	0.52
1:E:223:TYR:O	1:E:226:ILE:N	2.43	0.52
2:F:156:GLY:HA2	2:F:159:LEU:HD13	1.91	0.52
3:G:24:MET:CG	3:G:109:GLU:HG2	2.40	0.52
3:G:85:TRP:O	3:G:87:THR:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:89:ASP:CB	3:G:92:VAL:HG22	2.26	0.52
5:N:3:UNK:O	5:N:7:UNK:CB	2.58	0.52
1:I:40:HIS:ND1	1:I:40:HIS:N	2.57	0.52
1:I:61:TRP:HE1	1:I:74:LEU:HD21	1.75	0.52
1:I:63:LYS:HB2	1:I:63:LYS:HZ2	1.75	0.52
1:I:173:PHE:O	1:I:174:LYS:HG2	2.10	0.52
1:I:316:LYS:CE	1:I:373:THR:HG23	2.40	0.52
2:J:107:ILE:HG21	3:K:119:TYR:OH	2.09	0.52
2:J:150:ALA:HA	2:J:234:PHE:HE2	1.73	0.52
2:J:151:VAL:HG22	2:J:237:TRP:NE1	2.24	0.52
5:O:13:UNK:O	5:O:17:UNK:CB	2.58	0.52
1:A:66:LEU:HD21	1:A:71:SER:O	2.10	0.52
1:A:144:HIS:HD1	1:A:163:TRP:NE1	2.07	0.52
1:A:223:TYR:O	1:A:226:ILE:N	2.43	0.52
1:A:393:TYR:O	1:A:394:ASP:C	2.52	0.52
2:B:13:PHE:CD1	2:B:19:ALA:HA	2.44	0.52
2:B:204:MET:C	2:B:206:GLU:OE2	2.53	0.52
3:C:56:PRO:C	3:C:58:PHE:N	2.68	0.52
3:C:102:ARG:CG	3:C:102:ARG:NH1	2.72	0.52
1:E:61:TRP:HE1	1:E:74:LEU:HD21	1.75	0.52
2:F:174:GLN:NE2	2:F:185:LEU:HD11	2.25	0.52
3:G:67:TRP:CD1	3:G:67:TRP:H	2.26	0.52
1:I:48:PHE:C	1:I:48:PHE:HD2	2.14	0.52
1:I:66:LEU:HD21	1:I:71:SER:O	2.10	0.52
1:I:79:HIS:CD2	1:I:80:VAL:N	2.77	0.52
1:I:199:HIS:CD2	2:J:106:TRP:HE1	2.28	0.52
2:J:82:ALA:CB	2:J:146:TYR:OH	2.55	0.52
2:J:119:PHE:HB3	2:J:123:LEU:CD2	2.38	0.52
2:J:235:LEU:HD23	2:J:236:TRP:N	2.24	0.52
1:A:54:LEU:HD21	1:A:80:VAL:HG13	1.91	0.52
1:A:92:LYS:O	1:A:122:SER:HA	2.09	0.52
1:A:198:TRP:C	1:A:200:PHE:H	2.17	0.52
1:A:207:ALA:HA	1:A:210:ILE:HB	1.91	0.52
1:A:299:LEU:HD21	1:A:417:ILE:CG2	2.40	0.52
3:C:80:LEU:HD23	3:C:159:ILE:HG22	1.91	0.52
1:E:44:SER:O	1:E:45:GLN:HG2	2.09	0.52
1:E:63:LYS:HB3	1:E:66:LEU:HG	1.91	0.52
1:E:276:GLN:C	1:E:278:PRO:CD	2.81	0.52
1:E:425:PHE:HB2	1:I:267:ARG:CZ	2.39	0.52
2:F:21:GLY:C	2:F:23:VAL:N	2.68	0.52
2:F:148:ILE:HG13	2:F:149:THR:H	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:106:VAL:O	3:G:107:LEU:C	2.52	0.52
1:I:173:PHE:HZ	1:I:175:ASP:HB2	1.72	0.52
5:O:3:UNK:O	5:O:7:UNK:CB	2.58	0.52
2:B:154:SER:O	2:B:157:TRP:HB3	2.09	0.51
2:B:240:GLY:C	2:B:243:TYR:H	2.17	0.51
3:C:114:TYR:N	3:C:160:MET:HE1	2.24	0.51
1:E:199:HIS:CD2	2:F:106:TRP:HE1	2.28	0.51
1:E:328:GLY:C	1:E:339:ASN:HB2	2.36	0.51
2:F:227:PHE:C	2:F:229:SER:H	2.16	0.51
4:H:509:UNK:O	4:H:513:UNK:CB	2.58	0.51
5:N:13:UNK:O	5:N:17:UNK:CB	2.58	0.51
1:I:179:LEU:O	1:I:180:LEU:C	2.52	0.51
1:I:213:TRP:HA	1:I:213:TRP:CE3	2.45	0.51
1:I:223:TYR:CE2	4:L:515:UNK:C	2.93	0.51
3:K:96:ALA:O	3:K:99:GLU:N	2.43	0.51
1:A:40:HIS:ND1	1:A:40:HIS:N	2.57	0.51
2:B:227:PHE:C	2:B:229:SER:H	2.16	0.51
3:C:106:VAL:O	3:C:107:LEU:C	2.52	0.51
1:E:144:HIS:HD1	1:E:163:TRP:NE1	2.07	0.51
1:E:219:ILE:O	1:E:220:ILE:HB	2.09	0.51
1:E:316:LYS:CE	1:E:373:THR:HG23	2.40	0.51
2:F:93:GLY:O	2:F:96:PHE:N	2.43	0.51
1:I:105:LEU:HB3	1:I:135:LEU:HB2	1.92	0.51
1:I:223:TYR:O	1:I:226:ILE:N	2.43	0.51
1:I:224:LEU:HD21	4:L:519:UNK:O	2.10	0.51
3:K:62:TRP:HZ2	3:K:144:PRO:HB3	1.73	0.51
3:K:132:TRP:NE1	3:K:144:PRO:HG2	2.24	0.51
3:K:161:ALA:C	3:K:163:GLY:H	2.17	0.51
4:L:509:UNK:O	4:L:513:UNK:CB	2.58	0.51
1:A:110:GLN:HG2	1:A:133:ILE:CG2	2.41	0.51
1:A:180:LEU:C	1:A:182:GLY:N	2.66	0.51
1:A:223:TYR:CE2	4:D:515:UNK:C	2.93	0.51
2:B:210:LEU:HD23	3:C:158:SER:OG	2.10	0.51
2:B:233:TYR:HD1	2:B:234:PHE:N	2.09	0.51
3:C:85:TRP:O	3:C:87:THR:N	2.42	0.51
3:C:96:ALA:O	3:C:99:GLU:N	2.43	0.51
5:M:1:UNK:H	5:M:4:UNK:CB	2.22	0.51
5:M:13:UNK:O	5:M:17:UNK:CB	2.58	0.51
1:E:79:HIS:HB2	1:E:128:ASP:OD2	2.10	0.51
1:E:202:TRP:HB3	2:F:130:VAL:CB	2.40	0.51
1:E:207:ALA:HA	1:E:210:ILE:CG1	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:220:ILE:C	1:E:222:SER:N	2.65	0.51
2:F:123:LEU:CD2	2:F:124:VAL:HG13	2.41	0.51
1:I:299:LEU:HD21	1:I:417:ILE:CG2	2.40	0.51
2:J:93:GLY:O	2:J:96:PHE:N	2.43	0.51
3:K:118:ILE:O	3:K:121:GLY:N	2.42	0.51
3:K:161:ALA:C	3:K:163:GLY:N	2.68	0.51
1:A:304:TYR:CE1	1:A:423:PRO:HB3	2.46	0.51
1:A:316:LYS:CE	1:A:373:THR:HG23	2.40	0.51
1:A:356:ASP:C	1:A:358:GLY:N	2.69	0.51
1:A:371:THR:O	1:A:372:LYS:HG3	2.10	0.51
3:C:62:TRP:HZ2	3:C:144:PRO:HB3	1.73	0.51
1:E:223:TYR:CE2	4:H:515:UNK:C	2.93	0.51
1:E:371:THR:O	1:E:372:LYS:HG3	2.10	0.51
1:E:397:SER:HB2	2:J:182:LEU:HD23	1.93	0.51
1:I:110:GLN:HG2	1:I:133:ILE:CG2	2.41	0.51
2:J:21:GLY:C	2:J:23:VAL:N	2.68	0.51
2:J:233:TYR:HD1	2:J:234:PHE:N	2.08	0.51
3:K:24:MET:CG	3:K:109:GLU:HG2	2.40	0.51
3:K:115:ALA:O	3:K:118:ILE:N	2.44	0.51
3:K:121:GLY:HA2	3:K:153:SER:OG	2.11	0.51
1:A:61:TRP:HE1	1:A:74:LEU:HD21	1.75	0.51
1:A:105:LEU:HD13	1:A:135:LEU:CD2	2.39	0.51
2:B:90:LEU:HD13	2:B:92:PHE:HB3	1.92	0.51
3:C:80:LEU:H	3:C:80:LEU:CD2	2.22	0.51
1:E:173:PHE:O	1:E:174:LYS:HG2	2.10	0.51
2:F:238:PHE:CD1	2:F:241:LYS:HB2	2.41	0.51
3:G:161:ALA:C	3:G:163:GLY:N	2.68	0.51
1:I:50:ARG:NH1	1:I:387:ARG:O	2.44	0.51
1:I:79:HIS:HB2	1:I:128:ASP:OD2	2.10	0.51
1:I:98:ALA:C	1:I:100:GLU:H	2.18	0.51
1:I:242:VAL:O	1:I:246:VAL:HG23	2.10	0.51
2:J:35:PHE:CD1	2:J:96:PHE:HE2	2.29	0.51
2:J:90:LEU:HD13	2:J:92:PHE:HB3	1.92	0.51
2:J:161:PHE:C	2:J:161:PHE:HD1	2.19	0.51
1:A:199:HIS:CD2	2:B:106:TRP:HE1	2.28	0.51
1:A:207:ALA:HA	1:A:210:ILE:CG1	2.41	0.51
2:B:169:ILE:HG22	2:B:170:ALA:H	1.75	0.51
2:B:248:VAL:O	2:B:248:VAL:HG12	2.11	0.51
3:C:90:ARG:C	3:C:92:VAL:H	2.19	0.51
1:E:62:SER:HB3	1:E:73:VAL:N	2.16	0.51
1:E:120:SER:OG	1:E:275:LEU:HG	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:213:PHE:HA	2:F:216:GLU:HB3	1.93	0.51
3:G:88:ARG:HG2	3:G:90:ARG:N	2.08	0.51
1:A:98:ALA:C	1:A:100:GLU:H	2.19	0.51
1:A:200:PHE:C	1:A:202:TRP:H	2.17	0.51
2:B:184:SER:C	2:B:186:ALA:N	2.67	0.51
3:C:66:LEU:C	3:C:68:THR:N	2.68	0.51
1:E:224:LEU:HD21	4:H:519:UNK:O	2.11	0.51
1:E:329:GLU:OE2	1:E:336:ARG:HD3	2.11	0.51
2:F:233:TYR:HD1	2:F:234:PHE:N	2.09	0.51
3:G:22:ARG:C	3:G:24:MET:N	2.66	0.51
3:G:90:ARG:C	3:G:92:VAL:H	2.19	0.51
1:I:219:ILE:HD11	2:J:27:ASP:CA	2.26	0.51
3:K:113:VAL:HB	3:K:160:MET:CE	2.35	0.51
1:A:50:ARG:NH1	1:A:387:ARG:O	2.44	0.51
1:A:107:ARG:HG2	2:B:191:PHE:O	2.11	0.51
1:A:379:GLN:O	1:A:380:ASP:HB2	2.11	0.51
1:A:407:SER:HB3	1:A:410:GLY:H	1.76	0.51
2:B:205:VAL:HG13	2:F:239:VAL:O	2.10	0.51
3:C:69:GLU:O	3:C:73:GLU:HG3	2.11	0.51
3:C:84:LEU:HD11	3:C:110:TRP:CH2	2.46	0.51
1:E:213:TRP:HA	1:E:213:TRP:CE3	2.45	0.51
1:E:213:TRP:HB3	2:F:90:LEU:HD21	1.93	0.51
2:F:161:PHE:C	2:F:161:PHE:HD1	2.19	0.51
1:I:329:GLU:OE2	1:I:336:ARG:HD3	2.11	0.51
2:J:38:VAL:HG13	2:J:39:LEU:N	2.25	0.51
2:J:123:LEU:CD2	2:J:124:VAL:HG13	2.41	0.51
2:J:202:ILE:O	2:J:204:MET:N	2.44	0.51
3:K:110:TRP:HB3	3:K:164:ALA:CB	2.41	0.51
1:A:107:ARG:HH12	2:B:194:VAL:HG11	1.76	0.51
1:A:224:LEU:HD21	4:D:519:UNK:O	2.11	0.51
1:A:352:TYR:O	1:A:382:ARG:CD	2.59	0.51
2:B:123:LEU:CD2	2:B:124:VAL:HG13	2.41	0.51
2:B:202:ILE:O	2:B:204:MET:N	2.44	0.51
2:B:235:LEU:C	2:B:235:LEU:CD2	2.79	0.51
1:E:66:LEU:HD21	1:E:71:SER:O	2.10	0.51
1:E:352:TYR:O	1:E:382:ARG:CD	2.59	0.51
2:F:108:ASN:HA	2:F:112:ASN:ND2	2.26	0.51
2:F:114:TRP:CZ3	2:F:118:TYR:HB3	2.46	0.51
2:F:202:ILE:O	2:F:204:MET:N	2.44	0.51
1:I:105:LEU:HD13	1:I:135:LEU:CD2	2.39	0.51
1:I:207:ALA:HA	1:I:210:ILE:CG1	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:95:THR:HG21	2:J:134:LEU:HD23	1.93	0.51
2:J:136:LEU:O	2:J:140:MET:HB2	2.11	0.51
2:J:202:ILE:CG2	2:J:203:ARG:N	2.74	0.51
3:K:110:TRP:C	3:K:112:VAL:H	2.19	0.51
1:A:328:GLY:C	1:A:339:ASN:HB2	2.36	0.51
2:B:35:PHE:C	2:B:37:ALA:H	2.18	0.51
2:B:68:VAL:O	2:B:69:VAL:C	2.53	0.51
2:B:161:PHE:C	2:B:161:PHE:HD1	2.19	0.51
2:B:174:GLN:NE2	2:B:185:LEU:HD11	2.25	0.51
3:C:22:ARG:C	3:C:24:MET:H	2.16	0.51
3:C:41:TYR:CD1	3:C:41:TYR:C	2.89	0.51
3:C:161:ALA:C	3:C:163:GLY:N	2.68	0.51
1:E:98:ALA:C	1:E:100:GLU:H	2.19	0.51
1:E:104:VAL:HG23	1:E:166:ILE:HD12	1.93	0.51
1:E:107:ARG:HH12	2:F:194:VAL:HG11	1.76	0.51
1:E:222:SER:HA	1:E:234:GLN:HE22	1.76	0.51
2:F:49:THR:CB	2:F:72:LEU:HD13	2.41	0.51
2:F:136:LEU:O	2:F:140:MET:HB2	2.11	0.51
2:F:202:ILE:CG2	2:F:203:ARG:N	2.74	0.51
3:G:69:GLU:O	3:G:73:GLU:HG3	2.11	0.51
3:G:84:LEU:HD11	3:G:110:TRP:CH2	2.46	0.51
5:N:17:UNK:O	5:N:21:UNK:CB	2.59	0.51
1:I:379:GLN:O	1:I:380:ASP:HB2	2.11	0.51
2:J:114:TRP:CZ3	2:J:118:TYR:HB3	2.46	0.51
2:J:248:VAL:O	2:J:248:VAL:HG12	2.11	0.51
3:K:69:GLU:O	3:K:73:GLU:HG3	2.11	0.51
1:A:63:LYS:HB3	1:A:66:LEU:HG	1.91	0.50
1:A:213:TRP:HB3	2:B:90:LEU:HD21	1.93	0.50
1:A:299:LEU:HD11	1:A:418:GLY:N	2.26	0.50
2:B:78:ALA:O	2:B:81:GLN:HB3	2.12	0.50
2:B:93:GLY:O	2:B:96:PHE:N	2.43	0.50
2:B:95:THR:HG21	2:B:134:LEU:HD23	1.93	0.50
2:B:202:ILE:CG2	2:B:203:ARG:N	2.74	0.50
1:E:50:ARG:NH1	1:E:387:ARG:O	2.44	0.50
1:E:299:LEU:HD21	1:E:417:ILE:CG2	2.40	0.50
1:E:354:LEU:C	1:E:354:LEU:HD12	2.36	0.50
2:F:248:VAL:HG12	2:F:248:VAL:O	2.11	0.50
3:G:121:GLY:HA2	3:G:153:SER:OG	2.11	0.50
1:I:275:LEU:CD2	1:I:276:GLN:H	2.24	0.50
1:I:352:TYR:O	1:I:382:ARG:CD	2.59	0.50
1:I:375:GLU:C	1:I:375:GLU:OE1	2.54	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:81:GLN:O	2:J:82:ALA:C	2.54	0.50
2:J:169:ILE:HG22	2:J:170:ALA:H	1.75	0.50
2:J:174:GLN:O	2:J:185:LEU:HG	2.11	0.50
2:J:184:SER:C	2:J:186:ALA:N	2.67	0.50
5:O:17:UNK:O	5:O:21:UNK:CB	2.59	0.50
1:A:66:LEU:HD11	1:A:72:MET:N	2.27	0.50
1:A:79:HIS:HB2	1:A:128:ASP:OD2	2.10	0.50
1:A:89:ALA:HB3	1:A:153:GLY:C	2.37	0.50
1:A:90:ASN:OD1	1:A:92:LYS:HB2	2.11	0.50
2:B:233:TYR:C	2:B:233:TYR:HD1	2.20	0.50
1:E:52:ARG:HG2	1:E:81:PHE:HE1	1.72	0.50
1:E:107:ARG:HG2	2:F:191:PHE:O	2.11	0.50
1:E:107:ARG:NH1	2:F:194:VAL:HG11	2.26	0.50
1:E:275:LEU:CD2	1:E:276:GLN:H	2.24	0.50
1:E:425:PHE:CD2	1:I:267:ARG:NE	2.79	0.50
2:F:233:TYR:C	2:F:233:TYR:HD1	2.20	0.50
3:G:62:TRP:C	3:G:64:SER:N	2.63	0.50
1:I:107:ARG:HG2	2:J:191:PHE:O	2.11	0.50
1:I:304:TYR:CE1	1:I:423:PRO:HB3	2.46	0.50
1:I:390:ASP:C	1:I:392:ALA:N	2.67	0.50
2:J:203:ARG:CB	2:J:207:ARG:HH21	2.12	0.50
2:J:213:PHE:HA	2:J:216:GLU:HB3	1.93	0.50
1:A:238:ASP:O	1:A:239:ASP:C	2.54	0.50
2:B:136:LEU:O	2:B:140:MET:HB2	2.11	0.50
2:B:166:TRP:CZ3	2:B:170:ALA:HA	2.46	0.50
2:B:175:ALA:CB	2:B:182:LEU:HD11	2.41	0.50
1:E:110:GLN:HG2	1:E:133:ILE:CG2	2.41	0.50
1:E:219:ILE:HD11	2:F:27:ASP:CA	2.26	0.50
1:E:299:LEU:HD11	1:E:417:ILE:CB	2.37	0.50
2:F:38:VAL:HG13	2:F:39:LEU:N	2.25	0.50
2:F:42:TYR:O	2:F:45:HIS:HB3	2.12	0.50
1:I:62:SER:HB3	1:I:73:VAL:N	2.16	0.50
1:I:354:LEU:HD12	1:I:354:LEU:C	2.36	0.50
1:I:407:SER:HB3	1:I:410:GLY:H	1.76	0.50
2:J:49:THR:CB	2:J:72:LEU:HD13	2.41	0.50
3:K:106:VAL:O	3:K:107:LEU:C	2.52	0.50
3:K:132:TRP:CE2	3:K:144:PRO:CG	2.95	0.50
1:A:104:VAL:HG23	1:A:166:ILE:HD12	1.93	0.50
1:A:277:LYS:HB2	1:I:83:ALA:HA	1.94	0.50
1:A:328:GLY:O	1:A:339:ASN:HB2	2.11	0.50
1:A:375:GLU:C	1:A:375:GLU:OE1	2.54	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:114:TRP:CZ3	2:B:118:TYR:HB3	2.46	0.50
1:E:375:GLU:OE1	1:E:375:GLU:C	2.54	0.50
1:I:106:VAL:CG1	1:I:107:ARG:H	2.22	0.50
1:I:120:SER:OG	1:I:275:LEU:HG	2.10	0.50
1:I:131:PHE:C	1:I:131:PHE:CD1	2.90	0.50
1:I:265:PHE:CD1	1:I:267:ARG:C	2.89	0.50
1:I:299:LEU:HD11	1:I:418:GLY:N	2.26	0.50
2:J:35:PHE:C	2:J:37:ALA:H	2.18	0.50
2:J:238:PHE:CG	2:J:239:VAL:N	2.77	0.50
3:K:41:TYR:CD1	3:K:41:TYR:C	2.89	0.50
1:A:120:SER:OG	1:A:275:LEU:HG	2.10	0.50
1:A:131:PHE:C	1:A:131:PHE:CD1	2.90	0.50
1:A:275:LEU:HA	1:A:276:GLN:OE1	2.12	0.50
1:A:354:LEU:HD12	1:A:355:ALA:N	2.27	0.50
2:B:35:PHE:CD1	2:B:96:PHE:HE2	2.29	0.50
2:B:52:ASP:HB3	2:B:55:PHE:CB	2.41	0.50
5:M:17:UNK:O	5:M:21:UNK:CB	2.59	0.50
1:E:304:TYR:CE1	1:E:423:PRO:HB3	2.46	0.50
1:E:354:LEU:HD12	1:E:355:ALA:N	2.27	0.50
2:F:95:THR:HG21	2:F:134:LEU:HD23	1.93	0.50
1:I:40:HIS:CD2	1:I:144:HIS:HB3	2.47	0.50
1:I:90:ASN:OD1	1:I:92:LYS:HB2	2.11	0.50
1:I:178:THR:O	2:J:176:THR:HG23	2.12	0.50
1:I:328:GLY:C	1:I:339:ASN:HB2	2.36	0.50
2:J:240:GLY:HA2	2:J:243:TYR:CB	2.42	0.50
3:K:118:ILE:HG12	3:K:157:TYR:CZ	2.46	0.50
1:A:275:LEU:CD2	1:A:276:GLN:H	2.24	0.50
1:A:339:ASN:C	1:A:341:ASP:N	2.69	0.50
1:A:354:LEU:HD12	1:A:354:LEU:C	2.36	0.50
2:B:81:GLN:O	2:B:82:ALA:C	2.54	0.50
3:C:110:TRP:C	3:C:112:VAL:H	2.19	0.50
1:E:105:LEU:CD2	1:E:135:LEU:HD13	2.37	0.50
1:E:106:VAL:CG1	1:E:107:ARG:H	2.22	0.50
1:E:356:ASP:C	1:E:358:GLY:N	2.69	0.50
2:F:81:GLN:O	2:F:82:ALA:C	2.54	0.50
2:F:131:VAL:CG2	2:F:164:ASN:HD22	2.25	0.50
2:F:174:GLN:O	2:F:185:LEU:HG	2.11	0.50
2:F:220:VAL:O	2:F:221:ALA:HB2	2.12	0.50
3:G:42:GLU:HA	3:G:62:TRP:CH2	2.47	0.50
1:I:104:VAL:HG23	1:I:166:ILE:HD12	1.93	0.50
1:I:157:ILE:HD12	1:I:157:ILE:N	2.17	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:52:ASP:HB3	2:J:55:PHE:CB	2.41	0.50
2:J:148:ILE:HG13	2:J:149:THR:H	1.75	0.50
1:A:107:ARG:NH2	2:B:191:PHE:CD1	2.70	0.50
1:A:178:THR:O	2:B:176:THR:HG23	2.12	0.50
1:A:265:PHE:CD1	1:A:267:ARG:C	2.89	0.50
2:B:131:VAL:CB	2:B:132:PRO:CD	2.90	0.50
2:B:131:VAL:CB	2:B:132:PRO:HD3	2.35	0.50
2:B:223:PHE:O	2:B:224:PHE:HB2	2.12	0.50
3:C:132:TRP:CE2	3:C:144:PRO:CG	2.95	0.50
1:E:72:MET:HE1	1:E:164:ILE:HG12	1.93	0.50
1:E:90:ASN:C	1:E:92:LYS:N	2.70	0.50
1:E:105:LEU:HB3	1:E:135:LEU:HB2	1.92	0.50
1:E:131:PHE:CD1	1:E:131:PHE:C	2.90	0.50
2:F:33:LEU:C	2:F:33:LEU:CD2	2.82	0.50
2:F:35:PHE:CD1	2:F:96:PHE:HE2	2.29	0.50
2:F:35:PHE:C	2:F:37:ALA:H	2.18	0.50
2:F:186:ALA:O	2:F:187:ASP:C	2.53	0.50
3:G:159:ILE:CA	3:G:162:VAL:HG22	2.41	0.50
1:I:72:MET:HE1	1:I:164:ILE:HG12	1.94	0.50
1:I:113:GLY:HA2	1:I:129:TYR:HD2	1.77	0.50
3:K:84:LEU:HD11	3:K:110:TRP:CH2	2.46	0.50
1:A:405:PHE:O	1:A:412:ARG:CA	2.60	0.50
2:B:131:VAL:CG2	2:B:164:ASN:HD22	2.25	0.50
3:C:44:ILE:CG2	3:C:45:TYR:N	2.63	0.50
1:E:90:ASN:OD1	1:E:92:LYS:HB2	2.11	0.50
1:E:112:ILE:O	1:E:113:GLY:C	2.54	0.50
1:E:191:GLY:O	1:E:194:ARG:N	2.45	0.50
2:F:91:PRO:HB3	2:F:141:LEU:HG	1.94	0.50
2:F:169:ILE:HG22	2:F:170:ALA:H	1.75	0.50
3:G:102:ARG:CG	3:G:102:ARG:NH1	2.72	0.50
2:J:35:PHE:O	2:J:37:ALA:N	2.41	0.50
2:J:143:SER:CB	2:J:148:ILE:HD12	2.39	0.50
2:J:211:ARG:NH2	3:K:158:SER:CA	2.58	0.50
2:J:220:VAL:O	2:J:221:ALA:HB2	2.12	0.50
1:A:72:MET:HE1	1:A:164:ILE:HG12	1.93	0.50
1:A:329:GLU:OE2	1:A:336:ARG:HD3	2.11	0.50
3:C:42:GLU:HA	3:C:62:TRP:CH2	2.47	0.50
3:C:118:ILE:HG12	3:C:157:TYR:CZ	2.46	0.50
1:E:265:PHE:CD1	1:E:267:ARG:C	2.89	0.50
2:F:166:TRP:CZ3	2:F:170:ALA:HA	2.46	0.50
3:G:89:ASP:HB3	3:G:92:VAL:CG2	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:154:TYR:O	3:G:155:PRO:C	2.54	0.50
1:I:112:ILE:O	1:I:113:GLY:C	2.54	0.50
2:J:131:VAL:CG2	2:J:164:ASN:HD22	2.25	0.50
3:K:29:ALA:C	3:K:31:LEU:H	2.20	0.50
3:K:42:GLU:HA	3:K:62:TRP:CH2	2.47	0.50
3:K:90:ARG:C	3:K:92:VAL:H	2.19	0.50
3:K:132:TRP:HA	3:K:132:TRP:CE3	2.47	0.50
1:A:112:ILE:O	1:A:113:GLY:C	2.54	0.49
1:A:150:ASN:ND2	1:A:156:PRO:CB	2.75	0.49
1:A:425:PHE:CD2	1:E:267:ARG:NE	2.80	0.49
2:B:42:TYR:O	2:B:45:HIS:HB3	2.12	0.49
1:E:107:ARG:NH2	2:F:191:PHE:CD1	2.71	0.49
1:E:150:ASN:ND2	1:E:156:PRO:CB	2.75	0.49
1:E:390:ASP:C	1:E:392:ALA:N	2.67	0.49
2:F:76:PHE:C	2:F:78:ALA:H	2.19	0.49
3:G:29:ALA:C	3:G:31:LEU:H	2.20	0.49
1:I:90:ASN:OD1	1:I:92:LYS:N	2.45	0.49
1:I:107:ARG:HH12	2:J:194:VAL:HG11	1.76	0.49
1:I:213:TRP:HB3	2:J:90:LEU:HD21	1.93	0.49
1:I:238:ASP:O	1:I:239:ASP:C	2.55	0.49
1:I:275:LEU:HA	1:I:276:GLN:OE1	2.12	0.49
2:J:75:THR:O	2:J:75:THR:CG2	2.59	0.49
2:J:166:TRP:CZ3	2:J:170:ALA:HA	2.46	0.49
3:K:108:VAL:O	3:K:108:VAL:CG1	2.57	0.49
1:A:191:GLY:O	1:A:194:ARG:N	2.45	0.49
1:A:367:ALA:O	1:A:370:GLU:HG2	2.12	0.49
2:B:108:ASN:HA	2:B:112:ASN:ND2	2.26	0.49
2:B:174:GLN:O	2:B:185:LEU:HG	2.11	0.49
2:B:211:ARG:NH1	3:C:157:TYR:CE1	2.80	0.49
3:C:31:LEU:HD11	3:C:35:TYR:CD1	2.39	0.49
3:C:111:LEU:HD12	3:C:111:LEU:H	1.77	0.49
3:C:121:GLY:HA2	3:C:153:SER:OG	2.11	0.49
3:C:159:ILE:CA	3:C:162:VAL:HG22	2.41	0.49
1:E:97:ASN:OD1	1:E:107:ARG:NH1	2.45	0.49
1:E:367:ALA:O	1:E:370:GLU:HG2	2.12	0.49
1:E:381:ALA:O	1:E:385:ILE:HG13	2.12	0.49
1:E:405:PHE:O	1:E:412:ARG:CA	2.60	0.49
2:F:43:HIS:CE1	2:F:105:GLU:HG2	2.47	0.49
2:F:85:TRP:C	2:F:85:TRP:CD1	2.87	0.49
2:F:227:PHE:C	2:F:229:SER:N	2.71	0.49
3:G:41:TYR:CD1	3:G:41:TYR:C	2.89	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:118:ILE:HG12	3:G:157:TYR:CZ	2.46	0.49
1:I:282:ILE:HG22	1:I:283:ILE:H	1.78	0.49
1:I:405:PHE:O	1:I:412:ARG:CA	2.60	0.49
2:J:76:PHE:C	2:J:78:ALA:H	2.19	0.49
2:J:108:ASN:HA	2:J:112:ASN:ND2	2.26	0.49
1:A:52:ARG:NH2	1:A:81:PHE:HE1	2.11	0.49
1:A:199:HIS:CD2	2:B:106:TRP:NE1	2.80	0.49
3:C:108:VAL:O	3:C:108:VAL:CG1	2.57	0.49
3:C:110:TRP:C	3:C:112:VAL:N	2.70	0.49
1:E:113:GLY:HA2	1:E:129:TYR:HD2	1.77	0.49
1:E:238:ASP:O	1:E:239:ASP:C	2.54	0.49
1:E:242:VAL:O	1:E:245:ILE:HB	2.13	0.49
2:F:42:TYR:C	2:F:42:TYR:CD2	2.90	0.49
2:F:205:VAL:HA	2:J:239:VAL:HB	1.94	0.49
3:G:62:TRP:HZ2	3:G:144:PRO:HB3	1.73	0.49
3:G:66:LEU:C	3:G:68:THR:N	2.68	0.49
3:G:110:TRP:HB3	3:G:164:ALA:CB	2.41	0.49
3:G:110:TRP:C	3:G:112:VAL:H	2.19	0.49
3:G:111:LEU:HD12	3:G:111:LEU:H	1.77	0.49
1:I:116:PHE:O	1:I:116:PHE:CG	2.64	0.49
1:I:406:PHE:CE1	1:I:412:ARG:HB3	2.47	0.49
2:J:42:TYR:O	2:J:45:HIS:HB3	2.12	0.49
2:J:103:ILE:O	2:J:107:ILE:HG13	2.12	0.49
2:J:233:TYR:C	2:J:233:TYR:HD1	2.20	0.49
3:K:66:LEU:C	3:K:68:THR:N	2.68	0.49
1:A:49:LEU:O	1:A:53:THR:HG22	2.12	0.49
1:A:107:ARG:NH1	2:B:194:VAL:HG11	2.26	0.49
1:A:116:PHE:CG	1:A:116:PHE:O	2.64	0.49
1:A:137:ALA:HB1	1:A:166:ILE:CG2	2.42	0.49
1:A:214:PHE:HE2	2:B:28:TRP:CD1	2.30	0.49
1:A:282:ILE:HG22	1:A:283:ILE:H	1.77	0.49
2:B:81:GLN:C	2:B:83:PHE:N	2.71	0.49
2:B:103:ILE:O	2:B:107:ILE:HG13	2.12	0.49
3:C:29:ALA:C	3:C:31:LEU:H	2.20	0.49
1:E:89:ALA:HB3	1:E:153:GLY:C	2.37	0.49
1:E:221:ALA:O	1:E:225:ARG:CB	2.61	0.49
1:E:328:GLY:O	1:E:339:ASN:HB2	2.11	0.49
1:E:395:THR:O	1:I:272:GLN:NE2	2.46	0.49
2:F:175:ALA:CB	2:F:182:LEU:HD11	2.41	0.49
2:F:243:TYR:CD2	2:F:247:LYS:NZ	2.81	0.49
1:I:97:ASN:OD1	1:I:107:ARG:NH1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:150:ASN:ND2	1:I:156:PRO:CB	2.75	0.49
1:I:328:GLY:O	1:I:339:ASN:HB2	2.11	0.49
1:I:381:ALA:O	1:I:385:ILE:HG13	2.12	0.49
1:I:393:TYR:N	1:I:393:TYR:HD2	2.08	0.49
2:J:43:HIS:CE1	2:J:105:GLU:HG2	2.47	0.49
2:J:91:PRO:HB3	2:J:141:LEU:HG	1.94	0.49
3:K:111:LEU:HD12	3:K:111:LEU:H	1.77	0.49
1:A:97:ASN:OD1	1:A:107:ARG:NH1	2.45	0.49
1:A:105:LEU:HB3	1:A:135:LEU:HB2	1.92	0.49
1:A:393:TYR:N	1:A:393:TYR:HD2	2.09	0.49
1:E:40:HIS:CD2	1:E:144:HIS:HB3	2.47	0.49
1:E:52:ARG:NH2	1:E:81:PHE:HE1	2.11	0.49
1:E:79:HIS:CD2	1:E:80:VAL:H	2.31	0.49
1:E:111:PHE:HB3	1:E:132:SER:O	2.13	0.49
1:E:202:TRP:HB3	2:F:130:VAL:HB	1.95	0.49
1:E:214:PHE:HE2	2:F:28:TRP:CD1	2.30	0.49
1:E:299:LEU:HD11	1:E:418:GLY:N	2.26	0.49
1:E:339:ASN:C	1:E:341:ASP:N	2.69	0.49
2:F:35:PHE:O	2:F:37:ALA:N	2.41	0.49
2:F:129:LEU:O	2:F:130:VAL:C	2.55	0.49
3:G:110:TRP:C	3:G:112:VAL:N	2.70	0.49
3:G:132:TRP:CE2	3:G:144:PRO:CG	2.95	0.49
1:I:199:HIS:CD2	2:J:106:TRP:NE1	2.80	0.49
1:I:354:LEU:HD12	1:I:355:ALA:N	2.27	0.49
1:A:81:PHE:HZ	1:A:418:GLY:HA3	1.77	0.49
1:A:163:TRP:H	1:A:163:TRP:HD1	1.61	0.49
1:A:179:LEU:H	1:A:179:LEU:CD2	2.00	0.49
1:A:222:SER:HA	1:A:234:GLN:HE22	1.76	0.49
2:B:42:TYR:C	2:B:42:TYR:CD2	2.90	0.49
2:B:240:GLY:HA2	2:B:243:TYR:CB	2.42	0.49
1:E:90:ASN:OD1	1:E:92:LYS:N	2.45	0.49
1:E:407:SER:HB3	1:E:410:GLY:H	1.76	0.49
2:F:69:VAL:N	2:F:70:PRO:CD	2.76	0.49
2:F:149:THR:HG22	2:F:234:PHE:CZ	2.47	0.49
2:F:150:ALA:O	2:F:154:SER:OG	2.26	0.49
2:F:213:PHE:HB3	2:J:147:VAL:CG1	2.43	0.49
3:G:124:PHE:HD2	3:G:125:PHE:CE1	2.31	0.49
1:I:90:ASN:C	1:I:92:LYS:N	2.69	0.49
1:I:307:PRO:HG2	1:I:308:GLY:N	2.18	0.49
2:J:148:ILE:O	2:J:152:VAL:HG22	2.13	0.49
3:K:110:TRP:C	3:K:112:VAL:N	2.70	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:169:LYS:HA	3:K:175:PHE:HB2	1.95	0.49
1:A:40:HIS:CD2	1:A:144:HIS:HB3	2.46	0.49
1:A:79:HIS:CD2	1:A:80:VAL:H	2.31	0.49
2:B:69:VAL:N	2:B:70:PRO:CD	2.76	0.49
3:C:110:TRP:HB3	3:C:164:ALA:CB	2.41	0.49
1:E:116:PHE:O	1:E:116:PHE:CG	2.64	0.49
1:E:137:ALA:HB1	1:E:166:ILE:CG2	2.42	0.49
1:E:199:HIS:CD2	2:F:106:TRP:NE1	2.80	0.49
1:E:210:ILE:CA	2:F:92:PHE:CE1	2.93	0.49
1:E:217:LYS:HD2	2:F:24:LYS:NZ	2.28	0.49
1:E:406:PHE:CE1	1:E:412:ARG:HB3	2.47	0.49
2:F:78:ALA:O	2:F:81:GLN:HB3	2.11	0.49
2:F:223:PHE:O	2:F:224:PHE:HB2	2.12	0.49
3:G:132:TRP:HA	3:G:132:TRP:CE3	2.47	0.49
1:I:107:ARG:NH1	2:J:194:VAL:HG11	2.26	0.49
1:I:222:SER:HA	1:I:234:GLN:HE22	1.76	0.49
1:I:356:ASP:C	1:I:358:GLY:N	2.69	0.49
2:J:68:VAL:O	2:J:69:VAL:C	2.53	0.49
2:J:81:GLN:C	2:J:83:PHE:N	2.71	0.49
2:J:149:THR:HG22	2:J:234:PHE:CZ	2.47	0.49
2:J:211:ARG:NH1	3:K:157:TYR:CE1	2.81	0.49
2:J:219:PRO:O	2:J:220:VAL:CG2	2.58	0.49
3:K:89:ASP:CB	3:K:92:VAL:HG22	2.26	0.49
3:K:103:ARG:HD3	3:K:171:ARG:O	2.13	0.49
1:A:106:VAL:CG1	1:A:107:ARG:H	2.22	0.49
1:A:124:GLU:OE1	1:A:125:VAL:N	2.37	0.49
1:A:217:LYS:HD2	2:B:24:LYS:NZ	2.28	0.49
1:A:381:ALA:O	1:A:385:ILE:HG13	2.12	0.49
1:A:393:TYR:CE1	2:F:249:ILE:HG21	2.48	0.49
2:B:76:PHE:C	2:B:78:ALA:H	2.19	0.49
2:B:102:LEU:N	2:B:102:LEU:HD12	2.28	0.49
2:B:220:VAL:O	2:B:221:ALA:HB2	2.12	0.49
1:E:275:LEU:HA	1:E:276:GLN:OE1	2.12	0.49
2:F:232:VAL:O	2:F:233:TYR:C	2.56	0.49
1:I:105:LEU:HD22	1:I:135:LEU:CD1	2.38	0.49
1:I:137:ALA:HB1	1:I:166:ILE:CG2	2.42	0.49
2:J:42:TYR:C	2:J:42:TYR:CD2	2.90	0.49
1:A:307:PRO:CG	1:A:308:GLY:H	2.18	0.49
1:A:352:TYR:O	1:A:382:ARG:HG2	2.13	0.49
1:A:395:THR:HG23	1:E:271:LEU:O	2.13	0.49
2:B:213:PHE:HA	2:B:216:GLU:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:124:PHE:HD2	3:C:125:PHE:CE1	2.31	0.49
1:E:66:LEU:HD11	1:E:72:MET:N	2.27	0.49
1:E:316:LYS:HE2	1:E:373:THR:CG2	2.43	0.49
1:E:352:TYR:O	1:E:382:ARG:HG2	2.13	0.49
2:F:65:TRP:CG	2:F:66:PRO:HD3	2.48	0.49
2:F:240:GLY:HA2	2:F:243:TYR:CB	2.42	0.49
1:I:52:ARG:NH2	1:I:81:PHE:HE1	2.11	0.49
1:I:63:LYS:CG	1:I:64:THR:H	2.12	0.49
1:I:124:GLU:OE1	1:I:125:VAL:HG23	2.12	0.49
1:I:316:LYS:HE2	1:I:373:THR:CG2	2.43	0.49
2:J:43:HIS:O	2:J:45:HIS:N	2.46	0.49
3:K:159:ILE:CA	3:K:162:VAL:HG22	2.41	0.49
1:A:111:PHE:HB3	1:A:132:SER:O	2.13	0.49
1:A:192:ILE:CD1	2:B:121:ILE:HD13	2.31	0.49
1:A:270:PRO:O	1:A:271:LEU:HD23	2.12	0.49
1:A:278:PRO:O	1:A:279:LEU:CB	2.61	0.49
2:B:48:LEU:CD1	2:B:48:LEU:N	2.76	0.49
2:B:150:ALA:O	2:B:151:VAL:C	2.56	0.49
3:C:115:ALA:O	3:C:118:ILE:N	2.44	0.49
1:E:49:LEU:O	1:E:53:THR:HG22	2.12	0.49
2:F:52:ASP:HB3	2:F:55:PHE:CB	2.41	0.49
3:G:153:SER:C	3:G:156:ILE:HB	2.38	0.49
1:I:49:LEU:O	1:I:53:THR:HG22	2.12	0.49
1:I:191:GLY:O	1:I:194:ARG:N	2.45	0.49
1:I:214:PHE:HE2	2:J:28:TRP:CD1	2.31	0.49
1:I:266:PRO:HG2	1:I:267:ARG:HD3	1.95	0.49
2:J:220:VAL:O	2:J:220:VAL:CG1	2.61	0.49
3:K:124:PHE:HD2	3:K:125:PHE:CE1	2.31	0.49
1:A:245:ILE:O	1:A:246:VAL:C	2.56	0.48
1:A:299:LEU:HD11	1:A:417:ILE:CB	2.37	0.48
2:B:43:HIS:O	2:B:45:HIS:N	2.46	0.48
1:E:81:PHE:HZ	1:E:418:GLY:HA3	1.77	0.48
1:E:150:ASN:OD1	1:E:156:PRO:HA	2.13	0.48
1:E:198:TRP:C	1:E:201:PRO:HD2	2.38	0.48
1:E:266:PRO:HG2	1:E:267:ARG:HD3	1.95	0.48
1:E:399:ILE:O	1:E:418:GLY:HA2	2.13	0.48
2:F:40:GLY:C	2:F:42:TYR:N	2.69	0.48
2:F:136:LEU:C	2:F:138:ILE:N	2.70	0.48
2:F:148:ILE:O	2:F:152:VAL:HG22	2.13	0.48
3:G:113:VAL:HB	3:G:160:MET:CE	2.35	0.48
1:I:66:LEU:HD11	1:I:72:MET:N	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:111:PHE:HB3	1:I:132:SER:O	2.13	0.48
1:I:226:ILE:O	1:I:231:ASP:OD2	2.31	0.48
2:J:78:ALA:O	2:J:81:GLN:HB3	2.12	0.48
3:K:64:SER:O	3:K:68:THR:HB	2.13	0.48
3:K:154:TYR:HB2	3:K:155:PRO:CD	2.40	0.48
1:A:124:GLU:OE1	1:A:125:VAL:HG23	2.12	0.48
1:A:305:LYS:HD2	1:A:308:GLY:HA3	1.94	0.48
1:A:328:GLY:N	1:A:339:ASN:ND2	2.61	0.48
1:A:406:PHE:CE1	1:A:412:ARG:HB3	2.47	0.48
2:B:43:HIS:CE1	2:B:105:GLU:HG2	2.47	0.48
2:B:227:PHE:C	2:B:229:SER:N	2.70	0.48
3:C:77:GLY:HA2	3:C:159:ILE:CG2	2.36	0.48
1:E:178:THR:O	2:F:176:THR:HG23	2.12	0.48
2:F:81:GLN:C	2:F:83:PHE:N	2.71	0.48
2:F:103:ILE:O	2:F:107:ILE:HG13	2.12	0.48
2:F:211:ARG:NH1	3:G:157:TYR:CE1	2.80	0.48
3:G:169:LYS:HA	3:G:175:PHE:HB2	1.95	0.48
1:I:211:LEU:O	1:I:212:TYR:C	2.57	0.48
1:I:217:LYS:HD2	2:J:24:LYS:NZ	2.28	0.48
1:I:242:VAL:O	1:I:245:ILE:HB	2.13	0.48
1:I:265:PHE:HD1	1:I:267:ARG:C	2.21	0.48
1:I:367:ALA:O	1:I:370:GLU:HG2	2.12	0.48
2:J:40:GLY:C	2:J:42:TYR:N	2.69	0.48
2:J:53:TRP:HB3	2:J:65:TRP:CD1	2.49	0.48
2:J:150:ALA:O	2:J:151:VAL:C	2.56	0.48
2:J:200:GLU:CG	2:J:201:TYR:N	2.75	0.48
2:J:238:PHE:HB2	2:J:241:LYS:NZ	2.28	0.48
1:A:104:VAL:HG23	1:A:166:ILE:CD1	2.44	0.48
1:A:198:TRP:C	1:A:201:PRO:HD2	2.38	0.48
1:A:266:PRO:HG2	1:A:267:ARG:HD3	1.95	0.48
1:A:339:ASN:C	1:A:341:ASP:H	2.21	0.48
1:A:390:ASP:C	1:A:392:ALA:N	2.68	0.48
2:B:65:TRP:CG	2:B:66:PRO:HD3	2.48	0.48
2:B:217:VAL:C	2:B:218:VAL:HG22	2.39	0.48
3:C:169:LYS:HA	3:C:175:PHE:HB2	1.95	0.48
1:E:139:ARG:CD	2:F:118:TYR:CE1	2.93	0.48
1:E:305:LYS:HD2	1:E:308:GLY:HA3	1.94	0.48
2:F:195:ARG:O	2:F:196:THR:HG23	2.13	0.48
1:I:81:PHE:HZ	1:I:418:GLY:HA3	1.77	0.48
1:I:89:ALA:HB3	1:I:153:GLY:C	2.37	0.48
1:I:105:LEU:CD2	1:I:135:LEU:HD13	2.37	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:198:TRP:C	1:I:201:PRO:HD2	2.38	0.48
1:I:399:ILE:O	1:I:418:GLY:HA2	2.13	0.48
2:J:217:VAL:C	2:J:218:VAL:HG22	2.39	0.48
2:J:223:PHE:O	2:J:224:PHE:HB2	2.12	0.48
3:K:73:GLU:OE2	3:K:155:PRO:HB2	2.13	0.48
1:A:211:LEU:O	1:A:212:TYR:C	2.56	0.48
1:A:221:ALA:O	1:A:225:ARG:CB	2.61	0.48
1:A:232:GLU:N	1:A:233:GLU:OE2	2.47	0.48
1:A:307:PRO:HG2	1:A:308:GLY:N	2.19	0.48
2:B:116:TRP:CD1	3:C:43:GLN:OE1	2.67	0.48
2:B:143:SER:CB	2:B:148:ILE:HD12	2.38	0.48
2:B:149:THR:HG22	2:B:234:PHE:CZ	2.47	0.48
3:C:73:GLU:OE2	3:C:155:PRO:HB2	2.13	0.48
3:C:153:SER:C	3:C:156:ILE:HB	2.38	0.48
1:E:245:ILE:O	1:E:246:VAL:C	2.56	0.48
1:E:270:PRO:O	1:E:271:LEU:HD23	2.12	0.48
1:E:379:GLN:O	1:E:380:ASP:HB2	2.11	0.48
2:F:61:ASP:OD2	2:F:65:TRP:HB3	2.13	0.48
2:F:91:PRO:O	2:F:137:ASP:CG	2.57	0.48
1:I:352:TYR:O	1:I:382:ARG:HG2	2.13	0.48
2:J:91:PRO:O	2:J:137:ASP:CG	2.57	0.48
2:J:143:SER:HB3	2:J:148:ILE:CD1	2.39	0.48
3:K:114:TYR:O	3:K:117:ALA:HB3	2.14	0.48
3:K:153:SER:C	3:K:156:ILE:HB	2.38	0.48
3:K:154:TYR:O	3:K:155:PRO:C	2.54	0.48
1:A:61:TRP:HZ2	1:A:161:GLY:HA2	1.79	0.48
1:A:90:ASN:OD1	1:A:92:LYS:N	2.45	0.48
1:A:139:ARG:O	1:A:140:ALA:O	2.32	0.48
1:A:188:GLU:O	1:A:188:GLU:OE2	2.31	0.48
2:B:43:HIS:C	2:B:45:HIS:N	2.70	0.48
2:B:57:VAL:HG22	2:B:125:PHE:CE2	2.48	0.48
3:C:64:SER:O	3:C:68:THR:HB	2.13	0.48
3:C:103:ARG:HD3	3:C:171:ARG:O	2.13	0.48
3:C:132:TRP:HA	3:C:132:TRP:CE3	2.47	0.48
3:C:140:THR:C	3:C:142:PHE:N	2.71	0.48
1:E:48:PHE:CZ	1:E:396:ASP:HB3	2.48	0.48
1:E:188:GLU:O	1:E:188:GLU:OE2	2.31	0.48
1:E:282:ILE:HG22	1:E:283:ILE:H	1.78	0.48
1:E:393:TYR:N	1:E:393:TYR:HD2	2.09	0.48
2:F:200:GLU:CG	2:F:201:TYR:N	2.75	0.48
2:F:238:PHE:HB2	2:F:241:LYS:NZ	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:77:GLY:HA2	3:G:159:ILE:CG2	2.36	0.48
3:G:103:ARG:HD3	3:G:171:ARG:O	2.13	0.48
3:G:106:VAL:O	3:G:109:GLU:CB	2.62	0.48
5:N:4:UNK:O	5:N:8:UNK:N	2.47	0.48
1:I:329:GLU:CG	1:I:338:LEU:HA	2.27	0.48
1:I:339:ASN:C	1:I:341:ASP:H	2.21	0.48
2:J:65:TRP:CG	2:J:66:PRO:HD3	2.48	0.48
2:J:90:LEU:CD2	2:J:92:PHE:HB3	2.44	0.48
2:J:207:ARG:O	2:J:212:THR:HG23	2.14	0.48
3:K:39:ARG:HA	3:K:42:GLU:OE2	2.14	0.48
1:A:202:TRP:HB3	2:B:130:VAL:HB	1.95	0.48
1:A:217:LYS:HD2	2:B:24:LYS:HZ3	1.78	0.48
1:A:242:VAL:O	1:A:245:ILE:HB	2.13	0.48
1:A:261:THR:CG2	2:B:170:ALA:HB3	2.43	0.48
2:B:129:LEU:O	2:B:130:VAL:C	2.55	0.48
2:B:136:LEU:C	2:B:138:ILE:N	2.70	0.48
2:B:200:GLU:CG	2:B:201:TYR:N	2.75	0.48
3:C:89:ASP:HB3	3:C:92:VAL:CG2	2.25	0.48
1:E:53:THR:HG23	1:E:157:ILE:HG21	1.96	0.48
2:F:35:PHE:CB	2:F:96:PHE:HE2	2.27	0.48
2:F:45:HIS:C	2:F:47:MET:N	2.71	0.48
2:F:90:LEU:CD2	2:F:92:PHE:HB3	2.44	0.48
1:I:61:TRP:HZ2	1:I:161:GLY:HA2	1.79	0.48
1:I:221:ALA:O	1:I:225:ARG:CB	2.61	0.48
1:I:305:LYS:HD2	1:I:308:GLY:HA3	1.94	0.48
2:J:195:ARG:O	2:J:196:THR:HG23	2.13	0.48
2:J:228:VAL:C	2:J:230:MET:N	2.64	0.48
5:O:4:UNK:O	5:O:8:UNK:N	2.47	0.48
1:A:150:ASN:OD1	1:A:156:PRO:HA	2.13	0.48
1:A:232:GLU:O	1:A:235:ILE:N	2.47	0.48
1:A:399:ILE:O	1:A:418:GLY:HA2	2.13	0.48
2:B:45:HIS:C	2:B:47:MET:N	2.71	0.48
2:B:61:ASP:OD2	2:B:65:TRP:HB3	2.13	0.48
2:B:207:ARG:O	2:B:212:THR:HG23	2.14	0.48
1:E:124:GLU:OE1	1:E:125:VAL:HG23	2.12	0.48
1:E:224:LEU:C	1:E:226:ILE:N	2.64	0.48
1:E:232:GLU:N	1:E:233:GLU:OE2	2.47	0.48
2:F:57:VAL:HG22	2:F:125:PHE:CE2	2.48	0.48
2:F:102:LEU:HD12	2:F:102:LEU:N	2.28	0.48
2:F:143:SER:HB3	2:F:148:ILE:CD1	2.39	0.48
2:F:172:LEU:HA	2:F:185:LEU:HD12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:195:ARG:HB2	2:F:196:THR:H	1.51	0.48
2:F:202:ILE:HG22	2:F:203:ARG:N	2.29	0.48
1:I:48:PHE:CZ	1:I:396:ASP:HB3	2.48	0.48
1:I:150:ASN:OD1	1:I:156:PRO:HA	2.12	0.48
1:I:188:GLU:O	1:I:188:GLU:OE2	2.31	0.48
1:I:202:TRP:HB3	2:J:130:VAL:HB	1.95	0.48
1:I:270:PRO:O	1:I:271:LEU:HD23	2.12	0.48
1:I:328:GLY:N	1:I:339:ASN:ND2	2.61	0.48
2:J:57:VAL:HG22	2:J:125:PHE:CE2	2.48	0.48
2:J:172:LEU:HA	2:J:185:LEU:HD12	1.96	0.48
2:J:175:ALA:CB	2:J:182:LEU:HD11	2.41	0.48
3:K:72:LEU:HA	3:K:75:VAL:HG12	1.96	0.48
3:K:106:VAL:O	3:K:109:GLU:CB	2.62	0.48
1:A:96:LEU:HD23	1:A:96:LEU:N	2.29	0.48
2:B:211:ARG:NH2	3:C:158:SER:CA	2.58	0.48
2:B:232:VAL:O	2:B:233:TYR:C	2.56	0.48
2:B:238:PHE:HB2	2:B:241:LYS:NZ	2.28	0.48
3:C:70:ILE:N	3:C:71:PRO:CD	2.77	0.48
1:E:54:LEU:CD2	1:E:80:VAL:HG13	2.44	0.48
1:E:105:LEU:HD13	1:E:135:LEU:CD2	2.39	0.48
1:E:196:TYR:OH	2:F:110:TYR:HE1	1.97	0.48
1:E:235:ILE:O	1:E:239:ASP:OD2	2.32	0.48
2:F:116:TRP:CD1	3:G:43:GLN:OE1	2.67	0.48
3:G:114:TYR:O	3:G:117:ALA:HB3	2.14	0.48
1:I:215:PHE:C	1:I:217:LYS:H	2.22	0.48
2:J:45:HIS:C	2:J:47:MET:N	2.71	0.48
2:J:90:LEU:C	2:J:92:PHE:N	2.72	0.48
3:K:31:LEU:HD11	3:K:35:TYR:CD1	2.39	0.48
1:A:48:PHE:CZ	1:A:396:ASP:HB3	2.48	0.48
1:A:282:ILE:HG22	1:A:283:ILE:N	2.29	0.48
2:B:40:GLY:C	2:B:42:TYR:N	2.69	0.48
2:B:53:TRP:HB3	2:B:65:TRP:CD1	2.49	0.48
2:B:75:THR:O	2:B:75:THR:CG2	2.59	0.48
2:B:90:LEU:CD2	2:B:92:PHE:HB3	2.44	0.48
2:B:91:PRO:O	2:B:137:ASP:CG	2.57	0.48
2:B:91:PRO:HB3	2:B:141:LEU:HG	1.94	0.48
2:B:200:GLU:O	2:B:201:TYR:HB2	2.14	0.48
3:C:65:ILE:HG23	5:M:7:UNK:CB	2.44	0.48
3:C:114:TYR:O	3:C:117:ALA:HB3	2.14	0.48
1:E:305:LYS:CG	1:E:310:GLU:H	2.22	0.48
1:E:328:GLY:N	1:E:339:ASN:ND2	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:43:HIS:O	2:F:45:HIS:N	2.46	0.48
2:F:182:LEU:HD12	2:F:183:MET:N	2.29	0.48
3:G:65:ILE:CG1	5:N:7:UNK:CB	2.91	0.48
3:G:73:GLU:OE2	3:G:155:PRO:HB2	2.13	0.48
2:J:136:LEU:C	2:J:138:ILE:N	2.70	0.48
3:K:22:ARG:C	3:K:24:MET:N	2.66	0.48
3:K:70:ILE:N	3:K:71:PRO:CD	2.77	0.48
1:A:148:GLN:CB	1:A:158:ILE:HG22	2.44	0.48
1:A:196:TYR:OH	2:B:110:TYR:HE1	1.97	0.48
1:A:223:TYR:HE2	4:D:515:UNK:C	2.27	0.48
2:B:81:GLN:O	2:B:83:PHE:N	2.47	0.48
2:B:103:ILE:O	2:B:103:ILE:HG22	2.14	0.48
3:C:39:ARG:HA	3:C:42:GLU:OE2	2.14	0.48
1:E:146:HIS:ND1	1:E:159:GLY:O	2.47	0.48
1:E:179:LEU:H	1:E:179:LEU:CD2	2.00	0.48
1:E:265:PHE:HD1	1:E:267:ARG:C	2.22	0.48
1:E:272:GLN:OE1	1:E:272:GLN:N	2.47	0.48
1:E:339:ASN:C	1:E:341:ASP:H	2.21	0.48
2:F:131:VAL:CB	2:F:132:PRO:CD	2.90	0.48
2:F:243:TYR:C	2:F:245:THR:N	2.52	0.48
3:G:70:ILE:N	3:G:71:PRO:CD	2.77	0.48
3:G:72:LEU:HA	3:G:75:VAL:HG12	1.96	0.48
1:I:54:LEU:CD2	1:I:80:VAL:HG13	2.44	0.48
1:I:79:HIS:CD2	1:I:80:VAL:H	2.31	0.48
1:I:272:GLN:N	1:I:272:GLN:OE1	2.47	0.48
2:J:69:VAL:N	2:J:70:PRO:CD	2.76	0.48
2:J:200:GLU:O	2:J:201:TYR:CB	2.61	0.48
3:K:109:GLU:O	3:K:112:VAL:HB	2.14	0.48
1:A:146:HIS:ND1	1:A:159:GLY:O	2.47	0.47
1:A:209:TRP:O	1:A:210:ILE:O	2.32	0.47
1:A:226:ILE:O	1:A:231:ASP:OD2	2.31	0.47
1:A:265:PHE:HD1	1:A:267:ARG:C	2.21	0.47
2:B:172:LEU:HA	2:B:185:LEU:HD12	1.96	0.47
2:B:195:ARG:O	2:B:196:THR:HG23	2.13	0.47
1:E:261:THR:CG2	2:F:170:ALA:HB3	2.43	0.47
1:E:329:GLU:HG3	1:E:338:LEU:CA	2.25	0.47
2:F:131:VAL:CB	2:F:132:PRO:HD3	2.35	0.47
2:F:150:ALA:O	2:F:151:VAL:C	2.56	0.47
2:F:217:VAL:C	2:F:218:VAL:HG22	2.39	0.47
3:G:65:ILE:HG23	5:N:7:UNK:CB	2.44	0.47
3:G:115:ALA:O	3:G:118:ILE:N	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:209:TRP:O	1:I:210:ILE:O	2.32	0.47
2:J:35:PHE:CB	2:J:96:PHE:HE2	2.27	0.47
2:J:97:ALA:O	2:J:98:VAL:C	2.57	0.47
2:J:102:LEU:N	2:J:102:LEU:HD12	2.28	0.47
2:J:116:TRP:CD1	3:K:43:GLN:OE1	2.67	0.47
2:J:129:LEU:O	2:J:130:VAL:C	2.55	0.47
2:J:232:VAL:O	2:J:233:TYR:C	2.56	0.47
2:J:240:GLY:CA	2:J:243:TYR:HB3	2.44	0.47
1:A:66:LEU:HD11	1:A:72:MET:CA	2.44	0.47
1:A:200:PHE:H	1:A:201:PRO:CD	2.27	0.47
1:A:272:GLN:N	1:A:272:GLN:OE1	2.47	0.47
2:B:71:ILE:O	2:B:72:LEU:C	2.56	0.47
2:B:93:GLY:O	2:B:96:PHE:HB3	2.14	0.47
2:B:148:ILE:O	2:B:152:VAL:HG22	2.13	0.47
2:B:245:THR:C	2:B:247:LYS:N	2.68	0.47
3:C:106:VAL:O	3:C:109:GLU:CB	2.62	0.47
1:E:55:ASN:OD1	1:E:401:GLY:HA2	2.14	0.47
1:E:226:ILE:O	1:E:231:ASP:OD2	2.31	0.47
1:E:232:GLU:O	1:E:235:ILE:N	2.47	0.47
1:E:270:PRO:HG2	1:E:272:GLN:OE1	2.14	0.47
1:E:282:ILE:HG22	1:E:283:ILE:N	2.29	0.47
2:F:150:ALA:HA	2:F:234:PHE:CE2	2.49	0.47
1:I:200:PHE:H	1:I:201:PRO:CD	2.27	0.47
1:I:312:THR:HG22	1:I:313:ILE:N	2.29	0.47
1:I:379:GLN:OE1	1:I:380:ASP:N	2.47	0.47
2:J:103:ILE:O	2:J:103:ILE:HG22	2.14	0.47
1:A:113:GLY:HA2	1:A:129:TYR:HD2	1.77	0.47
1:A:264:THR:HG21	2:B:171:ALA:HB2	1.96	0.47
2:B:220:VAL:O	2:B:220:VAL:CG1	2.61	0.47
3:C:65:ILE:CG1	5:M:7:UNK:CB	2.92	0.47
3:C:138:ARG:HB3	3:C:138:ARG:CZ	2.44	0.47
1:E:200:PHE:H	1:E:201:PRO:CD	2.27	0.47
1:E:215:PHE:C	1:E:217:LYS:H	2.22	0.47
2:F:203:ARG:HA	3:G:150:PHE:CZ	2.49	0.47
2:F:220:VAL:O	2:F:220:VAL:CG1	2.61	0.47
1:I:63:LYS:HG3	1:I:64:THR:N	2.14	0.47
1:I:235:ILE:O	1:I:239:ASP:OD2	2.32	0.47
1:I:270:PRO:HG2	1:I:272:GLN:OE1	2.14	0.47
1:I:339:ASN:C	1:I:341:ASP:N	2.69	0.47
2:J:71:ILE:O	2:J:72:LEU:C	2.56	0.47
2:J:120:PRO:O	2:J:122:SER:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:65:ILE:CG1	5:O:7:UNK:CB	2.91	0.47
1:A:139:ARG:CD	2:B:118:TYR:CE1	2.93	0.47
1:A:235:ILE:O	1:A:239:ASP:OD2	2.32	0.47
1:A:337:PHE:O	1:A:359:LEU:HB2	2.15	0.47
2:B:120:PRO:O	2:B:122:SER:N	2.47	0.47
2:B:240:GLY:CA	2:B:243:TYR:HB3	2.44	0.47
3:C:58:PHE:O	3:C:62:TRP:HB3	2.15	0.47
5:M:2:UNK:HA	5:M:5:UNK:CB	2.45	0.47
5:M:4:UNK:O	5:M:8:UNK:N	2.47	0.47
1:E:110:GLN:HG2	1:E:133:ILE:HG22	1.97	0.47
1:E:195:ILE:O	1:E:198:TRP:N	2.35	0.47
1:E:224:LEU:CD1	4:H:519:UNK:HA	2.42	0.47
1:E:340:PRO:C	1:E:342:VAL:H	2.21	0.47
2:F:43:HIS:C	2:F:45:HIS:N	2.70	0.47
2:F:184:SER:C	2:F:186:ALA:N	2.67	0.47
3:G:58:PHE:O	3:G:62:TRP:HB3	2.15	0.47
3:G:109:GLU:O	3:G:112:VAL:HB	2.14	0.47
5:N:2:UNK:HA	5:N:5:UNK:CB	2.45	0.47
1:I:96:LEU:HD23	1:I:96:LEU:N	2.29	0.47
1:I:146:HIS:ND1	1:I:159:GLY:O	2.47	0.47
1:I:232:GLU:O	1:I:235:ILE:N	2.47	0.47
1:I:315:VAL:HG11	1:I:403:LEU:HD11	1.96	0.47
2:J:48:LEU:CD1	2:J:48:LEU:N	2.76	0.47
3:K:58:PHE:O	3:K:62:TRP:HB3	2.15	0.47
1:A:55:ASN:OD1	1:A:401:GLY:HA2	2.14	0.47
1:A:207:ALA:C	1:A:209:TRP:H	2.23	0.47
1:A:214:PHE:CE1	2:B:31:LEU:HD22	2.50	0.47
1:A:312:THR:HG22	1:A:313:ILE:N	2.29	0.47
1:A:422:ILE:N	1:A:422:ILE:CD1	2.78	0.47
2:B:35:PHE:CB	2:B:96:PHE:HE2	2.27	0.47
2:B:57:VAL:HG22	2:B:125:PHE:HE2	1.80	0.47
3:C:75:VAL:O	3:C:79:ALA:N	2.47	0.47
1:E:123:LEU:CD1	1:E:123:LEU:H	2.28	0.47
1:E:207:ALA:C	1:E:209:TRP:H	2.23	0.47
1:E:313:ILE:HG22	1:E:314:GLN:N	2.30	0.47
2:F:53:TRP:HB3	2:F:65:TRP:CD1	2.49	0.47
2:F:97:ALA:O	2:F:98:VAL:C	2.57	0.47
2:F:188:LEU:O	2:F:191:PHE:N	2.48	0.47
3:G:64:SER:O	3:G:68:THR:HB	2.13	0.47
3:G:124:PHE:C	3:G:126:THR:N	2.73	0.47
1:I:104:VAL:HG23	1:I:166:ILE:CD1	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:139:ARG:O	1:I:140:ALA:O	2.32	0.47
1:I:146:HIS:ND1	1:I:160:PRO:C	2.73	0.47
1:I:207:ALA:C	1:I:209:TRP:H	2.23	0.47
2:J:61:ASP:OD2	2:J:65:TRP:HB3	2.13	0.47
2:J:131:VAL:CB	2:J:132:PRO:HD3	2.35	0.47
3:K:65:ILE:HG23	5:O:7:UNK:CB	2.44	0.47
3:K:75:VAL:O	3:K:79:ALA:N	2.47	0.47
5:O:2:UNK:HA	5:O:5:UNK:CB	2.45	0.47
1:A:379:GLN:OE1	1:A:380:ASP:N	2.47	0.47
2:B:114:TRP:CZ2	2:B:121:ILE:HD11	2.49	0.47
2:B:200:GLU:O	2:B:201:TYR:CB	2.61	0.47
2:B:202:ILE:HG22	2:B:203:ARG:N	2.29	0.47
3:C:154:TYR:O	3:C:155:PRO:C	2.54	0.47
1:E:139:ARG:O	1:E:140:ALA:O	2.32	0.47
1:E:214:PHE:CE1	2:F:31:LEU:HD22	2.50	0.47
1:E:312:THR:HG22	1:E:313:ILE:N	2.29	0.47
1:E:379:GLN:OE1	1:E:380:ASP:N	2.47	0.47
1:E:398:GLN:HA	1:E:420:PRO:HA	1.96	0.47
2:F:81:GLN:O	2:F:83:PHE:N	2.47	0.47
2:F:90:LEU:C	2:F:92:PHE:N	2.72	0.47
2:F:200:GLU:O	2:F:201:TYR:HB2	2.14	0.47
1:I:110:GLN:HG2	1:I:133:ILE:HG22	1.97	0.47
1:I:148:GLN:CB	1:I:158:ILE:HG22	2.44	0.47
1:I:198:TRP:HZ3	2:J:128:ALA:CB	2.28	0.47
1:I:216:LYS:O	1:I:217:LYS:O	2.33	0.47
1:I:245:ILE:O	1:I:246:VAL:C	2.56	0.47
1:I:299:LEU:HD11	1:I:417:ILE:CB	2.37	0.47
1:I:398:GLN:HA	1:I:420:PRO:HA	1.96	0.47
2:J:202:ILE:HG22	2:J:203:ARG:N	2.29	0.47
2:J:203:ARG:HA	3:K:150:PHE:CZ	2.49	0.47
1:A:110:GLN:HG2	1:A:133:ILE:HG22	1.97	0.47
1:A:219:ILE:O	1:A:221:ALA:N	2.48	0.47
1:A:266:PRO:CD	1:A:267:ARG:N	2.67	0.47
1:A:266:PRO:CG	1:A:267:ARG:N	2.78	0.47
1:A:340:PRO:C	1:A:342:VAL:H	2.21	0.47
1:A:398:GLN:HA	1:A:420:PRO:HA	1.96	0.47
2:B:27:ASP:OD2	2:B:27:ASP:C	2.57	0.47
2:B:97:ALA:O	2:B:98:VAL:C	2.57	0.47
2:B:188:LEU:O	2:B:191:PHE:N	2.48	0.47
2:B:236:TRP:CZ3	2:B:239:VAL:HG21	2.50	0.47
2:B:243:TYR:CD2	2:B:247:LYS:NZ	2.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:61:TRP:HZ2	1:E:161:GLY:HA2	1.79	0.47
1:E:66:LEU:HD11	1:E:72:MET:CA	2.44	0.47
1:E:146:HIS:ND1	1:E:160:PRO:C	2.73	0.47
1:E:209:TRP:O	1:E:210:ILE:O	2.32	0.47
1:E:307:PRO:HD3	1:E:426:VAL:HG22	1.97	0.47
1:E:422:ILE:N	1:E:422:ILE:CD1	2.78	0.47
2:F:71:ILE:O	2:F:72:LEU:C	2.56	0.47
2:F:93:GLY:O	2:F:96:PHE:HB3	2.14	0.47
2:F:99:SER:O	2:F:100:GLY:C	2.58	0.47
2:F:114:TRP:CZ2	2:F:121:ILE:HD11	2.49	0.47
2:F:120:PRO:CD	2:F:123:LEU:HD22	2.41	0.47
2:F:192:HIS:O	2:F:193:PHE:O	2.33	0.47
2:F:207:ARG:O	2:F:212:THR:HG23	2.14	0.47
2:F:240:GLY:CA	2:F:243:TYR:HB3	2.44	0.47
3:G:39:ARG:HA	3:G:42:GLU:OE2	2.14	0.47
1:I:42:GLU:CA	1:I:45:GLN:HE21	2.28	0.47
1:I:114:GLU:HG3	1:I:280:THR:CB	2.18	0.47
1:I:163:TRP:H	1:I:163:TRP:HD1	1.61	0.47
1:I:179:LEU:H	1:I:179:LEU:CD2	2.00	0.47
1:I:223:TYR:HE2	4:L:515:UNK:C	2.27	0.47
1:I:264:THR:HG21	2:J:171:ALA:HB2	1.96	0.47
1:I:266:PRO:CG	1:I:267:ARG:H	2.28	0.47
1:I:282:ILE:HG22	1:I:283:ILE:N	2.29	0.47
1:I:337:PHE:O	1:I:359:LEU:HB2	2.15	0.47
1:I:340:PRO:C	1:I:342:VAL:H	2.21	0.47
2:J:81:GLN:O	2:J:83:PHE:N	2.47	0.47
2:J:85:TRP:O	2:J:89:LYS:HA	2.15	0.47
2:J:114:TRP:CZ2	2:J:121:ILE:HD11	2.49	0.47
2:J:182:LEU:HD12	2:J:183:MET:N	2.29	0.47
3:K:153:SER:N	3:K:156:ILE:HD12	2.30	0.47
1:A:149:ILE:O	1:A:149:ILE:HG22	2.15	0.47
1:A:174:LYS:HB3	1:A:186:ASP:OD1	2.15	0.47
1:A:266:PRO:CG	1:A:267:ARG:H	2.28	0.47
2:B:151:VAL:HG22	2:B:237:TRP:HE1	1.80	0.47
2:B:216:GLU:OE2	2:B:216:GLU:CA	2.58	0.47
3:C:110:TRP:CE3	3:C:164:ALA:N	2.83	0.47
1:E:84:TRP:CZ2	1:E:91:PRO:HD3	2.50	0.47
1:E:216:LYS:O	1:E:217:LYS:O	2.33	0.47
1:E:223:TYR:HE2	4:H:515:UNK:C	2.27	0.47
3:G:110:TRP:CE3	3:G:164:ALA:N	2.83	0.47
1:I:53:THR:HG23	1:I:157:ILE:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:123:LEU:CD1	1:I:123:LEU:H	2.28	0.47
1:I:195:ILE:HG23	1:I:199:HIS:HB3	1.97	0.47
1:I:232:GLU:N	1:I:233:GLU:OE2	2.47	0.47
1:I:307:PRO:HD3	1:I:426:VAL:HG22	1.97	0.47
1:I:313:ILE:HG22	1:I:314:GLN:N	2.30	0.47
2:J:27:ASP:OD2	2:J:27:ASP:C	2.57	0.47
2:J:137:ASP:O	2:J:140:MET:HB3	2.15	0.47
3:K:148:ILE:C	3:K:152:MET:HB2	2.40	0.47
1:A:53:THR:HG23	1:A:157:ILE:HG21	1.96	0.47
1:A:57:TYR:CE1	1:A:77:LYS:HB2	2.50	0.47
1:A:114:GLU:HG3	1:A:280:THR:CB	2.18	0.47
1:A:195:ILE:O	1:A:198:TRP:N	2.35	0.47
1:A:198:TRP:HZ3	2:B:128:ALA:CB	2.28	0.47
2:B:162:TYR:HB3	2:B:163:PRO:CD	2.45	0.47
1:E:57:TYR:CE1	1:E:77:LYS:HB2	2.50	0.47
1:E:104:VAL:HG23	1:E:166:ILE:CD1	2.44	0.47
1:E:148:GLN:CB	1:E:158:ILE:HG22	2.44	0.47
1:E:198:TRP:HZ3	2:F:128:ALA:CB	2.28	0.47
1:E:399:ILE:CG1	1:E:400:GLY:H	2.23	0.47
2:F:27:ASP:OD2	2:F:27:ASP:C	2.57	0.47
2:F:120:PRO:O	2:F:122:SER:N	2.47	0.47
3:G:153:SER:N	3:G:156:ILE:HD12	2.30	0.47
1:I:139:ARG:CD	2:J:118:TYR:CE1	2.93	0.47
2:J:43:HIS:C	2:J:45:HIS:N	2.70	0.47
2:J:160:LEU:C	2:J:163:PRO:HG2	2.40	0.47
3:K:70:ILE:HA	3:K:70:ILE:HD13	1.79	0.47
3:K:100:GLU:C	3:K:102:ARG:N	2.72	0.47
1:A:48:PHE:HB2	1:A:394:ASP:CB	2.45	0.47
1:A:270:PRO:HG2	1:A:272:GLN:OE1	2.14	0.47
2:B:223:PHE:O	2:B:224:PHE:CB	2.63	0.47
3:C:109:GLU:O	3:C:112:VAL:HB	2.14	0.47
3:C:148:ILE:C	3:C:152:MET:HB2	2.40	0.47
3:C:154:TYR:HB2	3:C:155:PRO:CD	2.40	0.47
1:E:46:GLN:O	1:E:47:ALA:C	2.58	0.47
1:E:49:LEU:C	1:E:51:MET:N	2.73	0.47
1:E:96:LEU:HD23	1:E:96:LEU:N	2.29	0.47
1:E:330:TYR:HD1	1:E:402:LEU:O	1.98	0.47
1:E:337:PHE:O	1:E:359:LEU:HB2	2.15	0.47
2:F:162:TYR:HB3	2:F:163:PRO:CD	2.45	0.47
1:I:100:GLU:CD	1:I:105:LEU:HB2	2.40	0.47
1:I:174:LYS:HB3	1:I:186:ASP:OD1	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:330:TYR:HD1	1:I:402:LEU:O	1.98	0.47
2:J:65:TRP:CB	2:J:66:PRO:CD	2.93	0.47
2:J:90:LEU:HD22	2:J:92:PHE:HB3	1.97	0.47
2:J:236:TRP:CZ3	2:J:239:VAL:HG21	2.50	0.47
2:B:32:THR:HG22	2:B:33:LEU:N	2.30	0.46
2:B:150:ALA:HA	2:B:234:PHE:CE2	2.49	0.46
2:B:192:HIS:O	2:B:193:PHE:O	2.33	0.46
2:B:203:ARG:HA	3:C:150:PHE:CZ	2.49	0.46
3:C:72:LEU:HA	3:C:75:VAL:HG12	1.96	0.46
3:C:143:THR:O	3:C:147:ILE:HB	2.15	0.46
1:E:42:GLU:CA	1:E:45:GLN:HE21	2.28	0.46
1:E:66:LEU:HD22	1:E:70:GLU:C	2.40	0.46
1:E:278:PRO:O	1:E:279:LEU:CB	2.61	0.46
1:E:315:VAL:HG11	1:E:403:LEU:HD11	1.97	0.46
2:F:57:VAL:HG22	2:F:125:PHE:HE2	1.80	0.46
2:F:103:ILE:O	2:F:103:ILE:HG22	2.14	0.46
2:F:205:VAL:N	2:J:239:VAL:CG1	2.78	0.46
3:G:42:GLU:HB2	3:G:62:TRP:HH2	1.81	0.46
3:G:148:ILE:C	3:G:152:MET:HB2	2.40	0.46
1:I:48:PHE:HB2	1:I:394:ASP:CB	2.45	0.46
1:I:151:VAL:HG12	1:I:153:GLY:N	2.30	0.46
2:J:19:ALA:O	2:J:23:VAL:CG2	2.63	0.46
2:J:93:GLY:O	2:J:96:PHE:HB3	2.14	0.46
3:K:110:TRP:CE3	3:K:164:ALA:N	2.83	0.46
1:A:54:LEU:CD2	1:A:80:VAL:HG13	2.44	0.46
1:A:118:PRO:HA	2:B:191:PHE:CZ	2.51	0.46
1:A:220:ILE:HG21	2:B:23:VAL:HG13	1.97	0.46
2:B:19:ALA:O	2:B:23:VAL:CG2	2.63	0.46
2:B:233:TYR:O	2:B:236:TRP:N	2.48	0.46
1:E:219:ILE:O	1:E:221:ALA:N	2.48	0.46
2:F:85:TRP:O	2:F:89:LYS:HA	2.15	0.46
2:F:98:VAL:HG13	2:F:129:LEU:HB2	1.97	0.46
3:G:75:VAL:O	3:G:79:ALA:N	2.47	0.46
1:I:66:LEU:HD11	1:I:72:MET:CA	2.44	0.46
1:I:219:ILE:O	1:I:221:ALA:N	2.48	0.46
1:I:278:PRO:O	1:I:279:LEU:CB	2.61	0.46
1:I:304:TYR:CD2	1:I:383:TRP:HH2	2.33	0.46
2:J:39:LEU:O	2:J:40:GLY:C	2.59	0.46
1:A:84:TRP:CZ2	1:A:91:PRO:HD3	2.50	0.46
1:A:313:ILE:HG22	1:A:314:GLN:N	2.30	0.46
2:B:137:ASP:O	2:B:140:MET:HB3	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:182:LEU:HD12	2:B:183:MET:N	2.29	0.46
2:F:19:ALA:O	2:F:23:VAL:CG2	2.63	0.46
2:F:200:GLU:O	2:F:201:TYR:CB	2.61	0.46
2:F:205:VAL:HG22	2:J:239:VAL:C	2.40	0.46
2:F:233:TYR:O	2:F:236:TRP:N	2.48	0.46
1:I:138:ARG:HA	1:I:173:PHE:CG	2.51	0.46
1:I:261:THR:CG2	2:J:170:ALA:HB3	2.43	0.46
2:J:138:ILE:O	2:J:140:MET:N	2.48	0.46
2:J:200:GLU:O	2:J:201:TYR:HB2	2.14	0.46
2:J:227:PHE:C	2:J:229:SER:N	2.71	0.46
2:J:235:LEU:C	2:J:235:LEU:CD2	2.79	0.46
1:A:146:HIS:ND1	1:A:160:PRO:C	2.73	0.46
1:A:316:LYS:HE2	1:A:373:THR:CG2	2.43	0.46
1:A:330:TYR:HD1	1:A:402:LEU:O	1.98	0.46
2:B:49:THR:CB	2:B:72:LEU:HD13	2.41	0.46
3:C:99:GLU:CD	3:C:103:ARG:HE	2.24	0.46
3:C:153:SER:N	3:C:156:ILE:HD12	2.30	0.46
1:E:220:ILE:HG21	2:F:23:VAL:HG13	1.97	0.46
2:F:137:ASP:O	2:F:140:MET:HB3	2.14	0.46
2:F:140:MET:O	2:F:141:LEU:C	2.59	0.46
2:F:151:VAL:HG22	2:F:237:TRP:HE1	1.80	0.46
2:F:160:LEU:C	2:F:163:PRO:HG2	2.40	0.46
3:G:70:ILE:HD13	3:G:70:ILE:HA	1.78	0.46
1:I:61:TRP:CD1	1:I:74:LEU:HD22	2.51	0.46
1:I:383:TRP:HD1	1:I:388:LEU:HD12	1.78	0.46
2:J:150:ALA:O	2:J:154:SER:OG	2.26	0.46
2:J:162:TYR:HB3	2:J:163:PRO:CD	2.45	0.46
3:K:143:THR:O	3:K:147:ILE:HB	2.15	0.46
1:A:46:GLN:O	1:A:47:ALA:C	2.58	0.46
1:A:148:GLN:NE2	1:A:150:ASN:HD22	2.14	0.46
1:A:304:TYR:CD2	1:A:383:TRP:HH2	2.33	0.46
2:B:150:ALA:O	2:B:151:VAL:O	2.34	0.46
3:C:72:LEU:C	3:C:74:LEU:H	2.23	0.46
1:E:48:PHE:HB2	1:E:394:ASP:CB	2.45	0.46
1:E:51:MET:CE	1:E:388:LEU:HD13	2.45	0.46
1:E:100:GLU:CD	1:E:105:LEU:HB2	2.41	0.46
1:E:211:LEU:O	1:E:212:TYR:C	2.56	0.46
1:E:264:THR:HG21	2:F:171:ALA:HB2	1.96	0.46
2:F:90:LEU:HD22	2:F:92:PHE:HB3	1.97	0.46
2:F:150:ALA:O	2:F:151:VAL:O	2.34	0.46
2:F:242:TRP:CZ3	2:F:245:THR:HG21	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:143:THR:O	3:G:147:ILE:HB	2.15	0.46
1:I:46:GLN:O	1:I:47:ALA:C	2.58	0.46
1:I:55:ASN:OD1	1:I:401:GLY:HA2	2.14	0.46
1:I:214:PHE:CE1	2:J:31:LEU:HD22	2.50	0.46
1:I:266:PRO:CG	1:I:267:ARG:N	2.78	0.46
2:J:233:TYR:O	2:J:236:TRP:N	2.48	0.46
1:A:49:LEU:C	1:A:51:MET:N	2.73	0.46
1:A:59:VAL:HG21	1:A:160:PRO:CG	2.46	0.46
1:A:151:VAL:HG12	1:A:153:GLY:N	2.30	0.46
1:A:215:PHE:C	1:A:217:LYS:H	2.22	0.46
1:A:219:ILE:HD11	2:B:27:ASP:CA	2.26	0.46
1:A:315:VAL:HG11	1:A:403:LEU:HD11	1.97	0.46
2:B:99:SER:O	2:B:100:GLY:C	2.58	0.46
2:B:177:GLU:HG3	1:I:422:ILE:CG1	2.39	0.46
1:E:202:TRP:HB3	2:F:130:VAL:CG1	2.46	0.46
1:E:266:PRO:CG	1:E:267:ARG:H	2.28	0.46
2:F:75:THR:O	2:F:75:THR:CG2	2.58	0.46
2:F:108:ASN:HD21	3:G:128:GLN:N	2.14	0.46
2:F:236:TRP:CZ3	2:F:239:VAL:HG21	2.50	0.46
3:G:100:GLU:C	3:G:102:ARG:N	2.72	0.46
3:G:143:THR:HB	3:G:144:PRO:CD	2.41	0.46
1:I:59:VAL:HG21	1:I:160:PRO:CG	2.46	0.46
3:K:90:ARG:C	3:K:92:VAL:N	2.73	0.46
3:K:157:TYR:O	3:K:160:MET:HB2	2.16	0.46
1:A:51:MET:CE	1:A:388:LEU:HD13	2.45	0.46
2:B:86:GLU:CD	2:B:86:GLU:C	2.84	0.46
2:B:90:LEU:HD22	2:B:92:PHE:HB3	1.97	0.46
2:B:110:TYR:HB3	2:B:111:CYS:H	1.31	0.46
2:B:175:ALA:HB1	2:B:182:LEU:CD1	2.43	0.46
3:C:43:GLN:OE1	3:C:43:GLN:HA	2.15	0.46
3:C:69:GLU:HB3	3:C:152:MET:HE3	1.98	0.46
1:E:53:THR:CG2	1:E:157:ILE:HG21	2.46	0.46
1:E:240:ARG:HG3	1:E:241:ARG:H	1.81	0.46
2:F:135:TRP:CE2	2:F:139:ILE:HD11	2.51	0.46
2:F:211:ARG:NH2	3:G:158:SER:CA	2.58	0.46
2:F:237:TRP:HE3	2:F:238:PHE:N	2.13	0.46
1:I:186:ASP:O	1:I:190:TYR:HB2	2.16	0.46
1:I:214:PHE:HE2	2:J:28:TRP:HD1	1.64	0.46
2:J:175:ALA:HB1	2:J:182:LEU:CD1	2.43	0.46
3:K:43:GLN:OE1	3:K:43:GLN:HA	2.15	0.46
1:A:53:THR:CG2	1:A:157:ILE:HG21	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:LEU:CD1	1:A:135:LEU:HD13	2.45	0.46
1:A:214:PHE:HE2	2:B:28:TRP:HD1	1.64	0.46
2:B:13:PHE:CZ	2:B:22:CYS:O	2.69	0.46
2:B:65:TRP:C	2:B:67:THR:N	2.68	0.46
2:B:138:ILE:O	2:B:140:MET:N	2.48	0.46
2:B:231:MET:HE3	2:B:231:MET:HA	1.98	0.46
3:C:42:GLU:HB2	3:C:62:TRP:HH2	1.81	0.46
3:C:157:TYR:O	3:C:158:SER:C	2.58	0.46
1:E:119:ARG:HG2	1:E:274:GLY:N	2.24	0.46
1:E:187:LEU:C	1:E:189:THR:N	2.70	0.46
1:E:266:PRO:CG	1:E:267:ARG:N	2.78	0.46
2:F:138:ILE:O	2:F:140:MET:N	2.48	0.46
2:F:205:VAL:CG1	2:J:239:VAL:O	2.58	0.46
2:F:213:PHE:HD2	2:J:147:VAL:CG2	2.29	0.46
1:I:63:LYS:N	1:I:72:MET:HG3	2.21	0.46
1:I:192:ILE:CD1	2:J:121:ILE:HD13	2.31	0.46
1:I:240:ARG:HG3	1:I:241:ARG:H	1.81	0.46
2:J:33:LEU:HD23	2:J:34:LEU:N	2.31	0.46
2:J:88:PHE:O	2:J:90:LEU:HB2	2.16	0.46
2:J:150:ALA:HA	2:J:234:PHE:CE2	2.49	0.46
2:J:237:TRP:HE3	2:J:238:PHE:N	2.13	0.46
3:K:69:GLU:OE2	3:K:152:MET:HG2	2.16	0.46
1:A:61:TRP:CD1	1:A:74:LEU:HD22	2.51	0.46
1:A:123:LEU:CD1	1:A:123:LEU:H	2.28	0.46
1:A:186:ASP:O	1:A:190:TYR:HB2	2.16	0.46
1:A:202:TRP:HB3	2:B:130:VAL:CG1	2.46	0.46
1:A:216:LYS:O	1:A:217:LYS:O	2.33	0.46
1:A:219:ILE:HG12	2:B:30:PHE:HD2	1.81	0.46
1:A:329:GLU:CG	1:A:338:LEU:HA	2.27	0.46
2:B:85:TRP:O	2:B:89:LYS:HA	2.15	0.46
2:B:166:TRP:O	2:B:167:PRO:C	2.59	0.46
2:B:242:TRP:CZ3	2:B:245:THR:HG21	2.51	0.46
1:E:105:LEU:HA	1:E:136:LYS:O	2.16	0.46
1:E:174:LYS:HB3	1:E:186:ASP:OD1	2.15	0.46
1:E:219:ILE:HG12	2:F:30:PHE:HD2	1.81	0.46
1:E:366:LEU:HD12	1:E:366:LEU:HA	1.80	0.46
3:G:43:GLN:OE1	3:G:43:GLN:HA	2.15	0.46
3:G:72:LEU:C	3:G:74:LEU:H	2.23	0.46
1:I:202:TRP:HB3	2:J:130:VAL:CG1	2.46	0.46
1:I:399:ILE:CG1	1:I:400:GLY:H	2.23	0.46
2:J:108:ASN:HD21	3:K:128:GLN:N	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:135:TRP:CE2	2:J:139:ILE:HD11	2.51	0.46
2:J:242:TRP:CZ3	2:J:245:THR:HG21	2.51	0.46
3:K:42:GLU:HB2	3:K:62:TRP:HH2	1.80	0.46
3:K:72:LEU:C	3:K:74:LEU:H	2.23	0.46
3:K:95:VAL:CG1	3:K:96:ALA:N	2.79	0.46
1:A:105:LEU:HD23	1:A:137:ALA:N	2.31	0.46
1:A:307:PRO:HD3	1:A:426:VAL:HG22	1.97	0.46
1:A:328:GLY:N	1:A:405:PHE:HE1	2.14	0.46
2:B:33:LEU:HD23	2:B:34:LEU:N	2.31	0.46
2:B:98:VAL:HG13	2:B:129:LEU:HB2	1.97	0.46
2:B:160:LEU:C	2:B:163:PRO:HG2	2.40	0.46
3:C:90:ARG:C	3:C:92:VAL:N	2.73	0.46
1:E:40:HIS:N	1:E:40:HIS:HD1	2.14	0.46
1:E:118:PRO:HA	2:F:191:PHE:CZ	2.51	0.46
1:E:195:ILE:HG23	1:E:199:HIS:HB3	1.97	0.46
1:E:238:ASP:C	1:E:242:VAL:HG23	2.41	0.46
2:F:63:ARG:O	2:F:64:MET:C	2.59	0.46
2:F:245:THR:C	2:F:247:LYS:N	2.68	0.46
3:G:99:GLU:CD	3:G:103:ARG:HE	2.24	0.46
2:J:68:VAL:N	2:J:70:PRO:HD2	2.31	0.46
3:K:99:GLU:CD	3:K:103:ARG:HE	2.24	0.46
1:A:105:LEU:HA	1:A:136:LYS:O	2.16	0.45
1:A:195:ILE:HG23	1:A:199:HIS:HB3	1.97	0.45
1:A:209:TRP:O	1:A:210:ILE:C	2.59	0.45
1:A:264:THR:O	1:A:264:THR:CG2	2.63	0.45
1:A:312:THR:C	1:A:313:ILE:HG13	2.41	0.45
2:B:35:PHE:O	2:B:37:ALA:N	2.41	0.45
2:B:140:MET:O	2:B:141:LEU:C	2.59	0.45
2:B:237:TRP:HE3	2:B:238:PHE:N	2.14	0.45
1:E:105:LEU:HD23	1:E:137:ALA:N	2.31	0.45
1:E:209:TRP:HD1	2:F:92:PHE:HA	1.81	0.45
2:F:86:GLU:C	2:F:86:GLU:CD	2.84	0.45
2:F:111:CYS:O	2:F:115:GLY:N	2.49	0.45
2:F:195:ARG:HD3	3:G:134:MET:HE3	1.98	0.45
2:F:236:TRP:O	2:F:238:PHE:HD2	1.99	0.45
1:I:57:TYR:CE1	1:I:77:LYS:HB2	2.51	0.45
1:I:118:PRO:HA	2:J:191:PHE:CZ	2.51	0.45
1:I:136:LYS:O	1:I:137:ALA:C	2.59	0.45
1:I:149:ILE:O	1:I:149:ILE:HG22	2.15	0.45
2:J:57:VAL:HG22	2:J:125:PHE:HE2	1.80	0.45
2:J:63:ARG:O	2:J:64:MET:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:GLU:OE2	1:A:105:LEU:N	2.49	0.45
1:A:100:GLU:CD	1:A:105:LEU:HB2	2.40	0.45
1:A:200:PHE:CB	1:A:201:PRO:HD3	2.35	0.45
1:A:263:SER:C	1:A:265:PHE:N	2.59	0.45
1:A:407:SER:HB3	1:A:411:LYS:N	2.31	0.45
2:B:155:LEU:HD13	2:B:159:LEU:HD11	1.98	0.45
3:C:157:TYR:O	3:C:160:MET:HB2	2.16	0.45
1:E:61:TRP:CD1	1:E:74:LEU:HD22	2.51	0.45
1:E:105:LEU:HD22	1:E:135:LEU:CD1	2.38	0.45
1:E:214:PHE:HE2	2:F:28:TRP:HD1	1.64	0.45
1:E:312:THR:C	1:E:313:ILE:HG13	2.41	0.45
2:F:68:VAL:N	2:F:70:PRO:HD2	2.31	0.45
3:G:95:VAL:CG1	3:G:96:ALA:N	2.79	0.45
1:I:51:MET:CE	1:I:388:LEU:HD13	2.45	0.45
1:I:105:LEU:HD23	1:I:137:ALA:N	2.31	0.45
1:I:148:GLN:NE2	1:I:150:ASN:HD22	2.14	0.45
1:I:209:TRP:HD1	2:J:92:PHE:HA	1.81	0.45
1:I:224:LEU:CD1	4:L:519:UNK:HA	2.43	0.45
1:I:422:ILE:N	1:I:422:ILE:CD1	2.78	0.45
2:J:32:THR:HG22	2:J:33:LEU:N	2.30	0.45
2:J:86:GLU:C	2:J:86:GLU:CD	2.84	0.45
2:J:155:LEU:HD13	2:J:159:LEU:HD11	1.98	0.45
2:J:166:TRP:HE3	2:J:169:ILE:HG22	1.81	0.45
2:J:236:TRP:O	2:J:238:PHE:HD2	1.99	0.45
2:J:245:THR:C	2:J:247:LYS:N	2.68	0.45
3:K:152:MET:HB3	3:K:156:ILE:HD11	1.98	0.45
3:K:152:MET:SD	3:K:156:ILE:HD11	2.57	0.45
1:A:66:LEU:HD22	1:A:70:GLU:C	2.40	0.45
2:B:65:TRP:CB	2:B:66:PRO:CD	2.93	0.45
2:B:68:VAL:N	2:B:70:PRO:HD2	2.31	0.45
3:C:95:VAL:CG1	3:C:96:ALA:N	2.79	0.45
3:C:167:TYR:CD1	3:C:167:TYR:C	2.95	0.45
1:E:100:GLU:OE2	1:E:105:LEU:N	2.49	0.45
1:E:149:ILE:HG22	1:E:149:ILE:O	2.15	0.45
1:E:151:VAL:HG12	1:E:153:GLY:N	2.30	0.45
1:E:209:TRP:O	1:E:210:ILE:C	2.59	0.45
2:F:65:TRP:CB	2:F:66:PRO:CD	2.93	0.45
2:F:240:GLY:C	2:F:243:TYR:HB3	2.41	0.45
3:G:152:MET:HB3	3:G:156:ILE:CD1	2.46	0.45
1:I:66:LEU:HD22	1:I:70:GLU:C	2.40	0.45
1:I:84:TRP:CZ2	1:I:91:PRO:HD3	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:141:GLY:HA3	1:I:143:TRP:CH2	2.52	0.45
1:I:219:ILE:HG12	2:J:30:PHE:HD2	1.81	0.45
1:I:220:ILE:HG21	2:J:23:VAL:HG13	1.97	0.45
2:J:82:ALA:CB	2:J:231:MET:HE2	2.38	0.45
2:J:140:MET:O	2:J:141:LEU:C	2.59	0.45
1:A:105:LEU:HD22	1:A:135:LEU:CD1	2.38	0.45
1:A:152:GLU:OE1	1:A:153:GLY:N	2.49	0.45
2:B:219:PRO:O	2:B:220:VAL:CG2	2.58	0.45
4:D:505:UNK:O	4:D:507:UNK:N	2.50	0.45
1:E:63:LYS:N	1:E:72:MET:HG3	2.21	0.45
1:E:80:VAL:O	1:E:81:PHE:C	2.59	0.45
1:E:138:ARG:HA	1:E:173:PHE:CG	2.51	0.45
1:E:156:PRO:O	1:E:156:PRO:HG2	2.17	0.45
1:E:200:PHE:CB	1:E:201:PRO:HD3	2.35	0.45
1:E:304:TYR:CD2	1:E:383:TRP:HH2	2.33	0.45
1:E:407:SER:HB3	1:E:411:LYS:N	2.31	0.45
2:F:82:ALA:CB	2:F:231:MET:HE2	2.38	0.45
2:F:213:PHE:HB3	2:J:147:VAL:HG11	1.99	0.45
3:G:90:ARG:C	3:G:92:VAL:N	2.73	0.45
1:I:49:LEU:C	1:I:51:MET:N	2.73	0.45
1:I:53:THR:CG2	1:I:157:ILE:HG21	2.46	0.45
1:I:152:GLU:OE1	1:I:153:GLY:N	2.49	0.45
1:I:203:MET:HE3	2:J:102:LEU:CB	2.38	0.45
1:I:238:ASP:C	1:I:242:VAL:HG23	2.41	0.45
1:A:51:MET:HG2	1:A:51:MET:O	2.17	0.45
1:A:113:GLY:HA2	1:A:129:TYR:HB3	1.99	0.45
1:A:141:GLY:HA3	1:A:143:TRP:CH2	2.52	0.45
1:A:240:ARG:HG3	1:A:241:ARG:H	1.81	0.45
2:B:166:TRP:HE3	2:B:169:ILE:HG22	1.81	0.45
3:C:152:MET:HB3	3:C:156:ILE:HD11	1.98	0.45
1:E:152:GLU:OE1	1:E:153:GLY:N	2.49	0.45
1:E:243:GLY:O	1:E:244:ALA:C	2.59	0.45
2:F:33:LEU:HD23	2:F:34:LEU:N	2.31	0.45
2:F:219:PRO:O	2:F:220:VAL:CG2	2.58	0.45
3:G:157:TYR:O	3:G:158:SER:C	2.58	0.45
1:I:100:GLU:O	1:I:101:PRO:C	2.59	0.45
1:I:139:ARG:CZ	2:J:118:TYR:HE1	2.30	0.45
2:J:150:ALA:O	2:J:151:VAL:O	2.34	0.45
2:J:223:PHE:O	2:J:224:PHE:CB	2.63	0.45
1:A:62:SER:HB3	1:A:72:MET:HG2	1.99	0.45
1:A:90:ASN:C	1:A:92:LYS:N	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:ASP:C	1:A:242:VAL:HG23	2.41	0.45
2:B:39:LEU:O	2:B:40:GLY:C	2.59	0.45
2:B:63:ARG:O	2:B:64:MET:C	2.59	0.45
2:B:65:TRP:C	2:B:65:TRP:CD1	2.94	0.45
2:B:88:PHE:O	2:B:90:LEU:HB2	2.16	0.45
2:B:240:GLY:C	2:B:243:TYR:HB3	2.41	0.45
3:C:152:MET:HB3	3:C:156:ILE:CD1	2.46	0.45
1:E:62:SER:HB3	1:E:72:MET:HG2	1.99	0.45
2:F:39:LEU:O	2:F:40:GLY:C	2.59	0.45
2:F:86:GLU:OE1	2:F:86:GLU:HA	2.17	0.45
3:G:153:SER:CA	3:G:156:ILE:HB	2.46	0.45
1:I:51:MET:HG2	1:I:51:MET:O	2.17	0.45
1:I:100:GLU:OE2	1:I:105:LEU:N	2.49	0.45
2:J:55:PHE:CZ	2:J:113:PHE:CZ	3.03	0.45
2:J:98:VAL:HG13	2:J:129:LEU:HB2	1.97	0.45
2:J:240:GLY:C	2:J:243:TYR:HB3	2.41	0.45
1:A:139:ARG:CZ	2:B:118:TYR:HE1	2.30	0.45
1:A:151:VAL:HG12	1:A:153:GLY:H	1.81	0.45
1:A:210:ILE:CA	2:B:92:PHE:CE1	2.93	0.45
2:B:195:ARG:HD3	3:C:134:MET:HE3	1.98	0.45
3:C:42:GLU:CB	3:C:62:TRP:HH2	2.30	0.45
3:C:99:GLU:O	3:C:102:ARG:HB3	2.16	0.45
1:E:100:GLU:O	1:E:101:PRO:C	2.59	0.45
1:E:136:LYS:O	1:E:137:ALA:C	2.59	0.45
1:E:139:ARG:CZ	2:F:118:TYR:HE1	2.30	0.45
1:E:141:GLY:HA3	1:E:143:TRP:CH2	2.52	0.45
1:E:329:GLU:CG	1:E:338:LEU:HA	2.27	0.45
1:E:420:PRO:HB2	2:J:180:GLY:O	2.15	0.45
2:F:169:ILE:O	2:F:170:ALA:C	2.60	0.45
2:F:223:PHE:O	2:F:224:PHE:CB	2.63	0.45
3:G:34:PHE:CD2	3:G:35:TYR:N	2.85	0.45
3:G:125:PHE:HD2	3:G:148:ILE:HB	1.80	0.45
3:G:138:ARG:HB3	3:G:138:ARG:CZ	2.44	0.45
3:G:152:MET:SD	3:G:156:ILE:HD11	2.57	0.45
1:I:80:VAL:O	1:I:81:PHE:C	2.59	0.45
2:J:169:ILE:O	2:J:170:ALA:C	2.60	0.45
2:J:195:ARG:HD3	3:K:134:MET:HE3	1.98	0.45
3:K:152:MET:HB3	3:K:156:ILE:CD1	2.46	0.45
1:A:42:GLU:HA	1:A:45:GLN:CG	2.46	0.45
1:A:247:LEU:C	1:A:247:LEU:CD1	2.90	0.45
1:A:258:TYR:CD1	2:B:166:TRP:CD1	3.05	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:LEU:HD23	1:A:353:LEU:C	2.42	0.45
1:A:366:LEU:HA	1:A:370:GLU:OE2	2.17	0.45
2:B:23:VAL:C	2:B:25:THR:H	2.25	0.45
2:B:213:PHE:HB3	2:F:147:VAL:HG11	1.99	0.45
3:C:40:ILE:O	3:C:43:GLN:HB3	2.17	0.45
3:C:113:VAL:HB	3:C:160:MET:CE	2.35	0.45
1:E:203:MET:HE3	2:F:102:LEU:CB	2.38	0.45
1:E:298:GLU:CD	1:E:316:LYS:HB2	2.40	0.45
1:E:335:LEU:HD23	1:E:353:LEU:C	2.42	0.45
3:G:69:GLU:OE2	3:G:152:MET:HG2	2.16	0.45
3:G:91:ASN:HD22	3:G:91:ASN:C	2.25	0.45
3:G:108:VAL:O	3:G:108:VAL:CG1	2.56	0.45
3:G:157:TYR:O	3:G:160:MET:HB2	2.16	0.45
3:G:167:TYR:C	3:G:167:TYR:CD1	2.95	0.45
1:I:113:GLY:HA2	1:I:129:TYR:HB3	1.99	0.45
1:I:156:PRO:HG2	1:I:156:PRO:O	2.17	0.45
1:I:209:TRP:O	1:I:210:ILE:C	2.59	0.45
1:I:312:THR:C	1:I:313:ILE:HG13	2.41	0.45
1:I:335:LEU:HD23	1:I:353:LEU:C	2.42	0.45
1:I:407:SER:HB3	1:I:411:LYS:N	2.31	0.45
2:J:192:HIS:O	2:J:193:PHE:O	2.33	0.45
3:K:32:ASN:O	3:K:36:LEU:HB2	2.17	0.45
3:K:138:ARG:HB3	3:K:138:ARG:CZ	2.44	0.45
3:K:143:THR:HB	3:K:144:PRO:CD	2.41	0.45
5:O:8:UNK:O	5:O:12:UNK:N	2.50	0.45
1:A:138:ARG:HA	1:A:173:PHE:CG	2.51	0.45
1:A:156:PRO:HG2	1:A:156:PRO:O	2.17	0.45
1:A:295:VAL:HG23	1:A:413:TYR:CD2	2.52	0.45
2:B:135:TRP:CE2	2:B:139:ILE:HD11	2.51	0.45
3:C:152:MET:SD	3:C:156:ILE:HD11	2.57	0.45
1:E:59:VAL:HG21	1:E:160:PRO:CG	2.46	0.45
2:F:155:LEU:HD13	2:F:159:LEU:HD11	1.98	0.45
3:G:40:ILE:O	3:G:43:GLN:HB3	2.17	0.45
3:G:116:VAL:O	3:G:117:ALA:C	2.60	0.45
1:I:193:ASP:O	1:I:194:ARG:C	2.60	0.45
1:I:222:SER:O	1:I:225:ARG:HB3	2.17	0.45
1:I:298:GLU:CD	1:I:316:LYS:HB2	2.40	0.45
1:I:328:GLY:N	1:I:405:PHE:HE1	2.14	0.45
2:J:44:ILE:O	2:J:48:LEU:HD13	2.17	0.45
2:J:111:CYS:O	2:J:115:GLY:N	2.49	0.45
2:J:243:TYR:CD2	2:J:247:LYS:NZ	2.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:91:ASN:C	3:K:91:ASN:HD22	2.25	0.45
3:K:99:GLU:O	3:K:102:ARG:HB3	2.16	0.45
1:A:225:ARG:O	1:A:231:ASP:CG	2.60	0.45
1:A:307:PRO:CD	1:A:426:VAL:HG22	2.47	0.45
2:B:169:ILE:HG23	2:B:170:ALA:N	2.32	0.45
3:C:34:PHE:CD2	3:C:35:TYR:N	2.85	0.45
3:C:69:GLU:OE2	3:C:152:MET:HG2	2.16	0.45
3:C:125:PHE:HD2	3:C:148:ILE:HB	1.80	0.45
3:C:169:LYS:HG2	3:C:175:PHE:O	2.17	0.45
1:E:163:TRP:H	1:E:163:TRP:HD1	1.61	0.45
1:E:170:MET:O	1:E:172:ASP:N	2.50	0.45
2:F:23:VAL:O	2:F:26:THR:HG22	2.17	0.45
2:F:212:THR:O	2:F:215:LYS:N	2.50	0.45
3:G:32:ASN:O	3:G:36:LEU:HB2	2.17	0.45
3:G:152:MET:HB3	3:G:156:ILE:HD11	1.98	0.45
1:I:170:MET:O	1:I:172:ASP:N	2.50	0.45
1:I:295:VAL:HG23	1:I:413:TYR:CD2	2.52	0.45
1:I:307:PRO:CD	1:I:426:VAL:HG22	2.47	0.45
2:J:86:GLU:OE1	2:J:86:GLU:HA	2.17	0.45
2:J:151:VAL:HG22	2:J:237:TRP:HE1	1.80	0.45
2:J:166:TRP:O	2:J:167:PRO:C	2.59	0.45
2:J:212:THR:O	2:J:215:LYS:N	2.50	0.45
3:K:35:TYR:OH	3:K:153:SER:HA	2.17	0.45
1:A:95:PHE:O	1:A:149:ILE:HA	2.17	0.44
1:A:243:GLY:O	1:A:244:ALA:C	2.59	0.44
2:B:42:TYR:HA	2:B:76:PHE:CZ	2.52	0.44
2:B:86:GLU:OE1	2:B:86:GLU:HA	2.17	0.44
2:B:108:ASN:HD21	3:C:128:GLN:N	2.14	0.44
3:C:147:ILE:HG22	3:C:148:ILE:HG13	1.99	0.44
1:E:105:LEU:HD13	1:E:135:LEU:CD1	2.45	0.44
2:F:55:PHE:CZ	2:F:113:PHE:CZ	3.03	0.44
2:F:213:PHE:CD2	2:J:147:VAL:HG22	2.53	0.44
3:G:99:GLU:O	3:G:102:ARG:HB3	2.16	0.44
3:G:147:ILE:HG22	3:G:148:ILE:HG13	1.99	0.44
1:I:105:LEU:HD13	1:I:135:LEU:CD1	2.45	0.44
1:I:271:LEU:HD23	1:I:271:LEU:N	2.31	0.44
1:I:315:VAL:HG11	1:I:403:LEU:CD1	2.48	0.44
1:I:417:ILE:HG13	1:I:418:GLY:H	1.82	0.44
1:A:63:LYS:HB2	1:A:63:LYS:NZ	2.32	0.44
1:A:209:TRP:HD1	2:B:92:PHE:HA	1.81	0.44
1:E:148:GLN:NE2	1:E:150:ASN:HD22	2.14	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:200:PHE:CE2	1:E:204:ILE:HD11	2.53	0.44
2:F:65:TRP:C	2:F:65:TRP:CD1	2.94	0.44
2:F:88:PHE:O	2:F:90:LEU:HB2	2.16	0.44
2:F:166:TRP:O	2:F:167:PRO:C	2.59	0.44
3:G:39:ARG:HA	3:G:42:GLU:HG2	1.98	0.44
1:I:105:LEU:HA	1:I:136:LYS:O	2.16	0.44
1:I:146:HIS:HA	1:I:161:GLY:CA	2.48	0.44
2:J:42:TYR:HA	2:J:76:PHE:CZ	2.53	0.44
2:J:231:MET:HE3	2:J:231:MET:HA	1.98	0.44
3:K:68:THR:HG21	5:O:8:UNK:N	2.32	0.44
3:K:169:LYS:HG2	3:K:175:PHE:O	2.17	0.44
1:A:223:TYR:C	1:A:223:TYR:HD1	2.25	0.44
1:A:417:ILE:HG13	1:A:418:GLY:H	1.82	0.44
2:B:203:ARG:H	2:B:203:ARG:HG3	1.65	0.44
3:C:42:GLU:OE2	3:C:125:PHE:CE2	2.70	0.44
3:C:91:ASN:C	3:C:91:ASN:HD22	2.25	0.44
5:M:8:UNK:O	5:M:12:UNK:N	2.50	0.44
1:E:95:PHE:O	1:E:149:ILE:HA	2.17	0.44
1:E:225:ARG:O	1:E:231:ASP:CG	2.60	0.44
1:E:247:LEU:C	1:E:247:LEU:CD1	2.90	0.44
1:E:366:LEU:HA	1:E:370:GLU:OE2	2.17	0.44
3:G:42:GLU:OE2	3:G:125:PHE:CE2	2.70	0.44
4:H:505:UNK:O	4:H:507:UNK:N	2.50	0.44
5:N:8:UNK:O	5:N:12:UNK:N	2.50	0.44
1:I:62:SER:HB3	1:I:72:MET:HG2	1.99	0.44
1:I:63:LYS:HB2	1:I:63:LYS:NZ	2.32	0.44
1:I:189:THR:O	1:I:189:THR:HG22	2.17	0.44
1:I:258:TYR:CD1	2:J:166:TRP:CD1	3.05	0.44
1:I:366:LEU:HA	1:I:370:GLU:OE2	2.17	0.44
3:K:77:GLY:HA2	3:K:159:ILE:CG2	2.36	0.44
1:A:100:GLU:OE2	1:A:105:LEU:CB	2.65	0.44
1:A:189:THR:O	1:A:189:THR:HG22	2.17	0.44
1:A:200:PHE:O	1:A:202:TRP:N	2.44	0.44
1:A:298:GLU:CD	1:A:316:LYS:HB2	2.40	0.44
1:A:352:TYR:CZ	1:A:386:GLU:HG2	2.53	0.44
2:B:169:ILE:O	2:B:170:ALA:C	2.60	0.44
3:C:39:ARG:HA	3:C:42:GLU:HG2	1.99	0.44
1:E:307:PRO:CD	1:E:426:VAL:HG22	2.47	0.44
2:F:231:MET:HA	2:F:231:MET:HE3	1.98	0.44
3:G:47:TRP:O	3:G:48:ARG:HB2	2.17	0.44
1:I:42:GLU:HA	1:I:45:GLN:CG	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:156:GLY:C	2:J:158:GLY:N	2.76	0.44
4:L:505:UNK:O	4:L:507:UNK:N	2.50	0.44
1:A:40:HIS:N	1:A:40:HIS:HD1	2.14	0.44
1:A:136:LYS:O	1:A:137:ALA:C	2.59	0.44
1:A:170:MET:O	1:A:172:ASP:N	2.50	0.44
1:A:224:LEU:CD1	4:D:519:UNK:HA	2.43	0.44
1:A:315:VAL:HG11	1:A:403:LEU:CD1	2.48	0.44
2:B:146:TYR:HD2	2:B:146:TYR:HA	1.50	0.44
2:B:171:ALA:C	2:B:173:HIS:H	2.25	0.44
2:B:200:GLU:CD	2:B:201:TYR:H	2.25	0.44
3:C:29:ALA:C	3:C:31:LEU:N	2.76	0.44
3:C:92:VAL:O	3:C:93:ASP:C	2.60	0.44
1:E:42:GLU:HB2	1:E:43:LYS:H	1.66	0.44
1:E:63:LYS:HB2	1:E:63:LYS:NZ	2.32	0.44
1:E:297:ALA:HB1	1:E:315:VAL:HG13	1.99	0.44
2:F:13:PHE:CZ	2:F:22:CYS:O	2.69	0.44
2:F:169:ILE:HG23	2:F:170:ALA:N	2.32	0.44
3:G:92:VAL:O	3:G:93:ASP:C	2.60	0.44
1:I:107:ARG:CG	2:J:191:PHE:CD1	3.00	0.44
1:I:199:HIS:HD2	2:J:106:TRP:NE1	2.16	0.44
2:J:169:ILE:HG23	2:J:170:ALA:N	2.32	0.44
3:K:42:GLU:OE2	3:K:125:PHE:CE2	2.70	0.44
3:K:72:LEU:O	3:K:75:VAL:HG12	2.18	0.44
3:K:107:LEU:C	3:K:109:GLU:N	2.76	0.44
3:K:118:ILE:O	3:K:119:TYR:C	2.60	0.44
3:K:167:TYR:CD1	3:K:167:TYR:C	2.95	0.44
1:A:100:GLU:O	1:A:101:PRO:C	2.59	0.44
1:A:191:GLY:C	1:A:193:ASP:N	2.74	0.44
1:A:332:ALA:C	1:A:334:GLY:H	2.26	0.44
1:A:390:ASP:O	1:A:392:ALA:N	2.51	0.44
2:B:23:VAL:O	2:B:26:THR:HG22	2.17	0.44
2:B:110:TYR:O	2:B:111:CYS:C	2.60	0.44
3:C:153:SER:CA	3:C:156:ILE:HB	2.46	0.44
1:E:51:MET:O	1:E:51:MET:HG2	2.17	0.44
1:E:105:LEU:CD1	1:E:135:LEU:HD22	2.43	0.44
1:E:186:ASP:O	1:E:190:TYR:HB2	2.16	0.44
1:E:200:PHE:O	1:E:202:TRP:N	2.44	0.44
1:E:295:VAL:HG23	1:E:413:TYR:CD2	2.52	0.44
1:E:315:VAL:HG11	1:E:403:LEU:CD1	2.48	0.44
2:F:44:ILE:O	2:F:48:LEU:HD13	2.17	0.44
2:F:93:GLY:O	2:F:94:ALA:C	2.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:110:TYR:HB3	2:F:111:CYS:H	1.31	0.44
2:F:151:VAL:HA	2:F:237:TRP:NE1	2.32	0.44
3:G:42:GLU:CB	3:G:62:TRP:HH2	2.30	0.44
3:G:104:HIS:O	3:G:108:VAL:N	2.50	0.44
1:I:86:GLN:HG3	1:I:87:ALA:N	2.32	0.44
1:I:225:ARG:O	1:I:231:ASP:CG	2.60	0.44
1:I:280:THR:HA	1:I:281:PRO:HD3	1.90	0.44
2:J:99:SER:O	2:J:100:GLY:C	2.58	0.44
2:J:120:PRO:CD	2:J:123:LEU:HD22	2.41	0.44
2:J:151:VAL:HA	2:J:237:TRP:NE1	2.32	0.44
3:K:24:MET:O	3:K:25:TRP:C	2.61	0.44
3:K:42:GLU:CB	3:K:62:TRP:HH2	2.30	0.44
3:K:153:SER:CA	3:K:156:ILE:HB	2.46	0.44
1:A:138:ARG:O	1:A:170:MET:HG3	2.17	0.44
1:A:277:LYS:HE3	1:I:84:TRP:HB3	1.99	0.44
2:B:53:TRP:CZ3	2:B:68:VAL:HG11	2.53	0.44
2:B:93:GLY:O	2:B:94:ALA:C	2.61	0.44
2:B:236:TRP:O	2:B:238:PHE:HD2	1.99	0.44
3:C:72:LEU:O	3:C:75:VAL:HG12	2.18	0.44
3:C:116:VAL:O	3:C:117:ALA:C	2.60	0.44
3:C:118:ILE:O	3:C:119:TYR:C	2.60	0.44
1:E:332:ALA:C	1:E:334:GLY:H	2.26	0.44
1:E:417:ILE:HG13	1:E:418:GLY:H	1.82	0.44
2:F:33:LEU:HD11	3:G:111:LEU:CB	2.48	0.44
3:G:68:THR:HG21	5:N:8:UNK:N	2.32	0.44
3:G:107:LEU:C	3:G:109:GLU:N	2.76	0.44
3:G:154:TYR:HB2	3:G:155:PRO:CD	2.40	0.44
3:G:159:ILE:C	3:G:162:VAL:HG22	2.42	0.44
1:I:95:PHE:O	1:I:149:ILE:HA	2.17	0.44
1:I:243:GLY:O	1:I:244:ALA:C	2.59	0.44
2:J:23:VAL:C	2:J:25:THR:H	2.25	0.44
2:J:23:VAL:O	2:J:26:THR:HG22	2.17	0.44
2:J:110:TYR:O	2:J:111:CYS:C	2.60	0.44
3:K:34:PHE:CD2	3:K:35:TYR:N	2.85	0.44
3:K:159:ILE:C	3:K:162:VAL:HG22	2.42	0.44
1:A:67:ASN:O	1:A:68:VAL:C	2.61	0.44
1:A:146:HIS:HA	1:A:161:GLY:CA	2.48	0.44
1:A:219:ILE:C	1:A:219:ILE:HD12	2.43	0.44
1:A:222:SER:O	1:A:225:ARG:HB3	2.17	0.44
2:B:105:GLU:O	2:B:107:ILE:N	2.51	0.44
2:B:212:THR:O	2:B:215:LYS:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:32:ASN:O	3:C:36:LEU:HB2	2.17	0.44
3:C:159:ILE:C	3:C:162:VAL:HG22	2.42	0.44
1:E:107:ARG:CG	2:F:191:PHE:CD1	3.00	0.44
1:E:265:PHE:CE1	1:E:268:THR:N	2.86	0.44
1:E:328:GLY:N	1:E:405:PHE:HE1	2.14	0.44
2:F:23:VAL:C	2:F:25:THR:H	2.25	0.44
2:F:143:SER:CB	2:F:148:ILE:HD12	2.39	0.44
3:G:72:LEU:O	3:G:75:VAL:HG12	2.18	0.44
1:I:40:HIS:N	1:I:40:HIS:HD1	2.14	0.44
1:I:107:ARG:O	2:J:192:HIS:CE1	2.71	0.44
1:I:138:ARG:O	1:I:170:MET:HG3	2.17	0.44
2:J:188:LEU:O	2:J:191:PHE:N	2.48	0.44
3:K:29:ALA:C	3:K:31:LEU:N	2.76	0.44
3:K:40:ILE:O	3:K:43:GLN:HB3	2.17	0.44
3:K:96:ALA:C	3:K:98:ARG:N	2.76	0.44
1:A:106:VAL:HG21	1:A:173:PHE:CZ	2.53	0.44
1:A:209:TRP:CZ3	1:A:246:VAL:HG11	2.53	0.44
3:C:68:THR:HG21	5:M:8:UNK:N	2.32	0.44
1:E:106:VAL:HG12	2:F:192:HIS:ND1	2.33	0.44
1:E:138:ARG:O	1:E:170:MET:HG3	2.17	0.44
1:E:146:HIS:ND1	1:E:161:GLY:N	2.66	0.44
1:E:199:HIS:HD2	2:F:106:TRP:NE1	2.16	0.44
1:E:209:TRP:CD1	2:F:92:PHE:HA	2.53	0.44
2:F:32:THR:HG22	2:F:33:LEU:N	2.30	0.44
2:F:110:TYR:O	2:F:111:CYS:C	2.60	0.44
2:F:166:TRP:HE3	2:F:169:ILE:HG22	1.81	0.44
2:F:200:GLU:CD	2:F:201:TYR:H	2.25	0.44
2:J:53:TRP:CZ3	2:J:68:VAL:HG11	2.53	0.44
3:K:157:TYR:O	3:K:158:SER:C	2.58	0.44
1:A:42:GLU:CA	1:A:45:GLN:HE21	2.28	0.43
1:A:209:TRP:CD1	2:B:92:PHE:HA	2.53	0.43
2:B:69:VAL:O	2:B:70:PRO:C	2.61	0.43
2:B:128:ALA:C	2:B:129:LEU:HG	2.43	0.43
2:B:138:ILE:O	2:B:142:LEU:HD13	2.18	0.43
2:B:177:GLU:CG	1:I:422:ILE:HG12	2.41	0.43
2:B:200:GLU:HG3	2:B:203:ARG:NH2	2.33	0.43
3:C:62:TRP:HZ2	3:C:144:PRO:CB	2.31	0.43
1:E:105:LEU:CD1	1:E:135:LEU:HD13	2.45	0.43
1:E:193:ASP:O	1:E:194:ARG:C	2.60	0.43
1:E:254:THR:C	1:E:256:ILE:N	2.75	0.43
2:F:105:GLU:O	2:F:107:ILE:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:45:TYR:O	3:G:49:ALA:HB3	2.18	0.43
3:G:118:ILE:O	3:G:119:TYR:C	2.60	0.43
3:G:169:LYS:HG2	3:G:175:PHE:O	2.17	0.43
1:I:100:GLU:OE2	1:I:105:LEU:CB	2.65	0.43
1:I:152:GLU:O	1:I:154:GLY:N	2.48	0.43
1:I:209:TRP:CZ3	1:I:246:VAL:HG11	2.53	0.43
1:I:375:GLU:OE1	1:I:375:GLU:O	2.36	0.43
1:I:390:ASP:O	1:I:392:ALA:N	2.51	0.43
2:J:33:LEU:HD11	3:K:111:LEU:CB	2.48	0.43
2:J:44:ILE:HD13	2:J:44:ILE:C	2.43	0.43
3:K:106:VAL:O	3:K:109:GLU:N	2.50	0.43
1:A:106:VAL:HG12	2:B:192:HIS:ND1	2.33	0.43
1:A:107:ARG:O	2:B:192:HIS:CE1	2.71	0.43
1:A:123:LEU:HD21	1:A:149:ILE:HG21	2.00	0.43
1:A:199:HIS:HD2	2:B:106:TRP:NE1	2.16	0.43
1:A:211:LEU:O	1:A:214:PHE:HB2	2.19	0.43
1:A:265:PHE:CE1	1:A:268:THR:N	2.86	0.43
1:A:271:LEU:HD23	1:A:271:LEU:N	2.31	0.43
2:B:77:ALA:HA	2:B:97:ALA:CB	2.48	0.43
3:C:35:TYR:OH	3:C:153:SER:HA	2.17	0.43
3:C:47:TRP:O	3:C:48:ARG:HB2	2.17	0.43
1:E:48:PHE:HB3	1:E:394:ASP:HB3	2.00	0.43
1:E:67:ASN:O	1:E:68:VAL:C	2.61	0.43
1:E:151:VAL:HG12	1:E:153:GLY:H	1.81	0.43
1:E:258:TYR:CD1	2:F:166:TRP:CD1	3.05	0.43
1:E:367:ALA:HB1	1:E:368:PRO:HD2	2.00	0.43
1:E:375:GLU:OE1	1:E:375:GLU:O	2.36	0.43
1:E:390:ASP:O	1:E:392:ALA:N	2.51	0.43
2:F:44:ILE:HD13	2:F:44:ILE:C	2.43	0.43
2:F:44:ILE:CG2	2:F:45:HIS:N	2.81	0.43
5:N:1:UNK:O	5:N:5:UNK:N	2.51	0.43
1:I:67:ASN:O	1:I:68:VAL:C	2.61	0.43
1:I:106:VAL:HG21	1:I:173:PHE:CZ	2.53	0.43
1:I:146:HIS:ND1	1:I:161:GLY:N	2.66	0.43
1:I:223:TYR:C	1:I:223:TYR:HD1	2.25	0.43
2:J:65:TRP:C	2:J:65:TRP:CD1	2.95	0.43
3:K:45:TYR:O	3:K:49:ALA:HB3	2.18	0.43
3:K:100:GLU:OE1	3:K:173:PRO:HG3	2.18	0.43
5:O:1:UNK:O	5:O:5:UNK:N	2.51	0.43
1:A:86:GLN:HG3	1:A:87:ALA:N	2.32	0.43
1:A:108:THR:O	1:A:109:ALA:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:VAL:CB	1:A:425:PHE:HA	2.48	0.43
1:A:340:PRO:C	1:A:342:VAL:N	2.77	0.43
1:A:381:ALA:CB	1:A:385:ILE:HD11	2.48	0.43
2:B:44:ILE:CG2	2:B:45:HIS:N	2.81	0.43
2:B:123:LEU:HD23	2:B:124:VAL:N	2.32	0.43
3:C:61:TYR:HE2	5:M:2:UNK:N	2.16	0.43
1:E:74:LEU:CG	1:E:147:ALA:HB2	2.48	0.43
1:E:163:TRP:CD1	1:E:163:TRP:N	2.86	0.43
1:E:189:THR:HG22	1:E:189:THR:O	2.17	0.43
1:E:199:HIS:HD2	2:F:106:TRP:CE2	2.36	0.43
1:E:209:TRP:CZ3	1:E:246:VAL:HG11	2.53	0.43
1:E:313:ILE:HG22	1:E:314:GLN:H	1.83	0.43
3:G:47:TRP:C	3:G:51:LEU:HD11	2.43	0.43
1:I:80:VAL:O	1:I:81:PHE:O	2.36	0.43
1:I:265:PHE:CE1	1:I:268:THR:N	2.86	0.43
1:I:340:PRO:C	1:I:342:VAL:N	2.77	0.43
1:I:381:ALA:CB	1:I:385:ILE:HD11	2.48	0.43
2:J:123:LEU:HD23	2:J:124:VAL:N	2.32	0.43
2:J:138:ILE:O	2:J:142:LEU:HD13	2.18	0.43
2:J:171:ALA:C	2:J:173:HIS:H	2.25	0.43
3:K:147:ILE:HG22	3:K:148:ILE:HG13	1.99	0.43
1:A:80:VAL:O	1:A:81:PHE:C	2.59	0.43
1:A:119:ARG:HG2	1:A:274:GLY:N	2.24	0.43
1:A:193:ASP:O	1:A:194:ARG:C	2.60	0.43
1:A:393:TYR:HB2	1:A:394:ASP:H	1.68	0.43
1:A:404:MET:CE	1:A:414:ALA:HB2	2.49	0.43
2:B:151:VAL:HA	2:B:237:TRP:NE1	2.32	0.43
3:C:45:TYR:O	3:C:49:ALA:HB3	2.18	0.43
3:C:45:TYR:CE1	3:C:61:TYR:HB3	2.54	0.43
1:E:191:GLY:C	1:E:193:ASP:N	2.74	0.43
1:E:419:GLY:HA2	1:E:420:PRO:HD3	1.81	0.43
2:F:42:TYR:HA	2:F:76:PHE:CZ	2.52	0.43
2:F:53:TRP:CZ3	2:F:68:VAL:HG11	2.53	0.43
2:F:62:ARG:NH1	2:F:249:ILE:HD12	2.34	0.43
2:F:77:ALA:HA	2:F:97:ALA:CB	2.48	0.43
2:F:200:GLU:HG3	2:F:203:ARG:NH2	2.33	0.43
1:I:219:ILE:C	1:I:219:ILE:HD12	2.43	0.43
1:I:297:ALA:HB1	1:I:315:VAL:HG13	1.99	0.43
1:I:313:ILE:HG22	1:I:314:GLN:H	1.83	0.43
2:J:40:GLY:O	2:J:41:GLY:C	2.61	0.43
2:J:61:ASP:OD2	2:J:65:TRP:CB	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:77:ALA:HA	2:J:97:ALA:CB	2.48	0.43
2:J:200:GLU:HG3	2:J:203:ARG:NH2	2.33	0.43
3:K:53:SER:HA	3:K:58:PHE:CD1	2.54	0.43
3:K:116:VAL:O	3:K:117:ALA:C	2.60	0.43
1:A:61:TRP:CZ2	1:A:161:GLY:HA2	2.53	0.43
1:A:297:ALA:HB1	1:A:315:VAL:HG13	1.99	0.43
1:A:305:LYS:CG	1:A:310:GLU:H	2.22	0.43
1:A:364:THR:HG22	1:A:372:LYS:HZ1	1.81	0.43
1:A:425:PHE:CG	1:E:267:ARG:HD2	2.53	0.43
2:B:192:HIS:O	2:B:193:PHE:C	2.62	0.43
3:C:100:GLU:OE1	3:C:173:PRO:HG3	2.19	0.43
1:E:61:TRP:CZ2	1:E:161:GLY:HA2	2.53	0.43
1:E:80:VAL:O	1:E:81:PHE:O	2.36	0.43
1:E:100:GLU:OE2	1:E:105:LEU:CB	2.65	0.43
1:E:123:LEU:HD21	1:E:149:ILE:HG21	2.00	0.43
1:E:364:THR:HG22	1:E:372:LYS:HZ1	1.82	0.43
2:F:40:GLY:O	2:F:41:GLY:C	2.61	0.43
2:F:156:GLY:C	2:F:158:GLY:N	2.76	0.43
3:G:29:ALA:C	3:G:31:LEU:N	2.76	0.43
3:G:167:TYR:HD1	3:G:168:ALA:N	2.17	0.43
1:I:151:VAL:HG12	1:I:153:GLY:H	1.81	0.43
1:I:200:PHE:CE2	1:I:204:ILE:HD11	2.53	0.43
1:I:303:VAL:HG12	1:I:304:TYR:N	2.34	0.43
1:I:352:TYR:CZ	1:I:386:GLU:HG2	2.53	0.43
2:J:105:GLU:O	2:J:107:ILE:N	2.51	0.43
2:J:128:ALA:C	2:J:129:LEU:HG	2.43	0.43
2:J:200:GLU:CD	2:J:201:TYR:H	2.25	0.43
3:K:39:ARG:HA	3:K:42:GLU:HG2	1.99	0.43
3:K:92:VAL:O	3:K:93:ASP:C	2.60	0.43
1:A:107:ARG:CG	2:B:191:PHE:CD1	3.00	0.43
1:A:146:HIS:ND1	1:A:161:GLY:N	2.66	0.43
1:A:178:THR:HG1	1:A:184:THR:HA	1.83	0.43
1:A:200:PHE:CE2	1:A:204:ILE:HD11	2.53	0.43
1:A:356:ASP:O	1:A:358:GLY:N	2.37	0.43
2:B:74:VAL:C	2:B:76:PHE:N	2.76	0.43
2:B:239:VAL:CG1	2:J:205:VAL:N	2.82	0.43
3:C:53:SER:HA	3:C:58:PHE:CD1	2.54	0.43
3:C:167:TYR:HD1	3:C:168:ALA:N	2.17	0.43
5:M:1:UNK:O	5:M:5:UNK:N	2.51	0.43
1:E:108:THR:O	1:E:109:ALA:HB2	2.18	0.43
1:E:113:GLY:HA2	1:E:129:TYR:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:352:TYR:CZ	1:E:386:GLU:HG2	2.53	0.43
2:F:61:ASP:OD2	2:F:65:TRP:CB	2.66	0.43
1:I:79:HIS:HE1	1:I:416:GLU:OE2	2.02	0.43
1:I:105:LEU:CD1	1:I:135:LEU:HD22	2.43	0.43
1:I:173:PHE:HE2	1:I:188:GLU:HG3	1.83	0.43
1:I:271:LEU:C	1:I:272:GLN:OE1	2.62	0.43
2:J:15:SER:C	2:J:17:ALA:H	2.26	0.43
2:J:176:THR:CG2	2:J:177:GLU:N	2.81	0.43
1:A:80:VAL:O	1:A:81:PHE:O	2.36	0.43
2:B:55:PHE:CZ	2:B:113:PHE:CZ	3.03	0.43
2:B:118:TYR:CD1	2:B:118:TYR:N	2.87	0.43
2:B:155:LEU:O	2:B:159:LEU:HD12	2.19	0.43
1:E:79:HIS:HE1	1:E:416:GLU:OE2	2.02	0.43
1:E:146:HIS:HA	1:E:161:GLY:CA	2.48	0.43
3:G:96:ALA:C	3:G:98:ARG:H	2.27	0.43
1:I:106:VAL:HG12	2:J:192:HIS:ND1	2.33	0.43
1:I:407:SER:O	1:I:408:PRO:C	2.62	0.43
2:J:13:PHE:CZ	2:J:22:CYS:O	2.69	0.43
2:J:44:ILE:HG12	3:K:126:THR:CG2	2.46	0.43
1:A:157:ILE:H	1:A:157:ILE:CD1	2.13	0.43
1:A:248:ALA:HA	1:A:251:ILE:CG2	2.49	0.43
1:A:272:GLN:NE2	1:I:395:THR:O	2.51	0.43
2:B:15:SER:C	2:B:17:ALA:H	2.26	0.43
2:B:61:ASP:OD2	2:B:65:TRP:CB	2.66	0.43
3:C:18:ILE:O	3:C:18:ILE:HG22	2.18	0.43
1:E:106:VAL:HG21	1:E:173:PHE:CZ	2.53	0.43
1:E:219:ILE:HD12	1:E:219:ILE:C	2.43	0.43
2:F:74:VAL:C	2:F:76:PHE:N	2.76	0.43
2:F:171:ALA:C	2:F:173:HIS:H	2.25	0.43
2:F:192:HIS:O	2:F:193:PHE:C	2.62	0.43
1:I:191:GLY:C	1:I:193:ASP:N	2.74	0.43
1:I:407:SER:C	1:I:409:SER:N	2.73	0.43
2:J:146:TYR:CZ	2:J:231:MET:CE	3.02	0.43
1:A:45:GLN:HB2	1:A:50:ARG:HD3	2.01	0.43
1:A:199:HIS:HD2	2:B:106:TRP:CE2	2.36	0.43
2:B:81:GLN:OE1	2:B:94:ALA:HB2	2.19	0.43
2:B:82:ALA:HB1	2:B:146:TYR:HH	1.77	0.43
2:B:156:GLY:C	2:B:158:GLY:N	2.76	0.43
3:C:47:TRP:C	3:C:51:LEU:HD11	2.43	0.43
1:E:152:GLU:O	1:E:154:GLY:N	2.48	0.43
1:E:195:ILE:C	1:E:197:ALA:N	2.76	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:222:SER:O	1:E:225:ARG:HB3	2.17	0.43
1:E:406:PHE:CE1	1:E:412:ARG:HG2	2.53	0.43
2:F:48:LEU:CD1	2:F:48:LEU:N	2.76	0.43
2:F:209:THR:OG1	2:J:237:TRP:CE2	2.72	0.43
3:G:168:ALA:O	3:G:172:ILE:HB	2.19	0.43
1:I:332:ALA:C	1:I:334:GLY:H	2.26	0.43
2:J:44:ILE:CG2	2:J:45:HIS:N	2.81	0.43
2:J:74:VAL:C	2:J:76:PHE:N	2.76	0.43
2:J:118:TYR:CD1	2:J:118:TYR:N	2.87	0.43
3:K:47:TRP:C	3:K:51:LEU:HD11	2.43	0.43
3:K:92:VAL:HG12	3:K:93:ASP:N	2.34	0.43
3:K:124:PHE:C	3:K:126:THR:N	2.73	0.43
3:K:132:TRP:NE1	3:K:144:PRO:CD	2.82	0.43
1:A:203:MET:HE3	2:B:102:LEU:CB	2.38	0.43
1:A:254:THR:C	1:A:256:ILE:N	2.75	0.43
1:A:406:PHE:HA	1:A:412:ARG:HA	2.01	0.43
2:B:40:GLY:O	2:B:41:GLY:C	2.60	0.43
2:B:40:GLY:C	2:B:42:TYR:H	2.27	0.43
2:B:68:VAL:CG1	2:B:72:LEU:HD12	2.49	0.43
2:B:101:LEU:HD12	2:B:105:GLU:HG3	2.01	0.43
1:E:191:GLY:O	1:E:192:ILE:C	2.61	0.43
1:E:381:ALA:CB	1:E:385:ILE:HD11	2.48	0.43
2:F:216:GLU:O	2:F:218:VAL:N	2.52	0.43
3:G:18:ILE:O	3:G:18:ILE:HG22	2.19	0.43
3:G:35:TYR:OH	3:G:153:SER:HA	2.18	0.43
3:G:85:TRP:O	3:G:88:ARG:HB3	2.19	0.43
3:G:92:VAL:HG12	3:G:93:ASP:N	2.34	0.43
1:I:108:THR:O	1:I:109:ALA:HB2	2.18	0.43
1:I:195:ILE:C	1:I:197:ALA:N	2.77	0.43
1:I:196:TYR:N	1:I:196:TYR:CD2	2.75	0.43
1:I:248:ALA:HA	1:I:251:ILE:CG2	2.49	0.43
1:I:269:ILE:HG13	2:J:184:SER:OG	2.19	0.43
1:I:425:PHE:CD2	1:I:425:PHE:N	2.80	0.43
2:J:82:ALA:HB1	2:J:146:TYR:HH	1.83	0.43
1:A:45:GLN:NE2	1:A:158:ILE:HD11	2.34	0.42
1:A:190:TYR:HD2	1:A:191:GLY:N	2.17	0.42
1:A:407:SER:O	1:A:408:PRO:C	2.62	0.42
2:B:44:ILE:O	2:B:48:LEU:HD13	2.17	0.42
2:B:80:ALA:O	2:B:83:PHE:HB3	2.19	0.42
2:B:150:ALA:O	2:B:154:SER:OG	2.26	0.42
2:B:216:GLU:O	2:B:218:VAL:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:96:ALA:C	3:C:98:ARG:N	2.76	0.42
1:E:45:GLN:HB2	1:E:50:ARG:HD3	2.01	0.42
1:E:104:VAL:HG11	1:E:143:TRP:NE1	2.34	0.42
1:E:173:PHE:HE2	1:E:188:GLU:HG3	1.84	0.42
1:E:248:ALA:HA	1:E:251:ILE:CG2	2.49	0.42
1:E:404:MET:CE	1:E:414:ALA:HB2	2.49	0.42
1:E:407:SER:C	1:E:409:SER:N	2.73	0.42
1:E:410:GLY:C	1:E:411:LYS:HG3	2.44	0.42
2:F:68:VAL:CG1	2:F:72:LEU:HD12	2.49	0.42
2:F:216:GLU:OE2	2:F:216:GLU:CA	2.58	0.42
3:G:41:TYR:CE1	3:G:62:TRP:CZ3	3.07	0.42
1:I:199:HIS:HD2	2:J:106:TRP:CE2	2.36	0.42
2:J:103:ILE:O	2:J:107:ILE:HD12	2.19	0.42
2:J:192:HIS:O	2:J:193:PHE:C	2.62	0.42
3:K:47:TRP:O	3:K:48:ARG:HB2	2.17	0.42
3:K:62:TRP:HZ2	3:K:144:PRO:CB	2.31	0.42
5:O:2:UNK:O	5:O:6:UNK:N	2.52	0.42
1:A:63:LYS:N	1:A:72:MET:HG3	2.21	0.42
1:A:104:VAL:HG11	1:A:143:TRP:NE1	2.34	0.42
1:A:187:LEU:C	1:A:189:THR:N	2.70	0.42
1:A:191:GLY:O	1:A:192:ILE:C	2.61	0.42
1:A:299:LEU:HD11	1:A:417:ILE:C	2.44	0.42
2:B:33:LEU:HD11	3:C:111:LEU:CB	2.48	0.42
2:B:146:TYR:CZ	2:B:231:MET:CE	3.02	0.42
2:B:239:VAL:HG12	2:J:205:VAL:CA	2.50	0.42
3:C:124:PHE:C	3:C:126:THR:N	2.73	0.42
1:E:107:ARG:O	2:F:192:HIS:CE1	2.71	0.42
1:E:299:LEU:HD11	1:E:417:ILE:C	2.44	0.42
2:F:203:ARG:H	2:F:203:ARG:HG3	1.65	0.42
3:G:24:MET:O	3:G:25:TRP:C	2.61	0.42
5:N:2:UNK:O	5:N:6:UNK:N	2.52	0.42
1:I:190:TYR:HD2	1:I:191:GLY:N	2.17	0.42
1:I:299:LEU:HD11	1:I:417:ILE:C	2.44	0.42
2:J:241:LYS:O	2:J:244:SER:OG	2.31	0.42
3:K:18:ILE:O	3:K:18:ILE:HG22	2.19	0.42
3:K:41:TYR:CE1	3:K:62:TRP:CZ3	3.07	0.42
3:K:85:TRP:O	3:K:88:ARG:HB3	2.19	0.42
1:A:48:PHE:CE2	1:A:49:LEU:HD23	2.54	0.42
1:A:48:PHE:HB3	1:A:394:ASP:HB3	2.00	0.42
1:A:74:LEU:CD1	1:A:147:ALA:HB2	2.49	0.42
1:A:279:LEU:HD23	1:A:279:LEU:HA	1.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:GLU:OE1	1:A:375:GLU:O	2.36	0.42
1:A:407:SER:HB3	1:A:411:LYS:H	1.85	0.42
2:B:62:ARG:NH1	2:B:249:ILE:HD12	2.34	0.42
2:B:117:THR:HG21	3:C:135:THR:HG21	2.01	0.42
2:B:225:SER:C	4:D:508:UNK:CB	2.93	0.42
3:C:92:VAL:HG12	3:C:93:ASP:N	2.34	0.42
3:C:115:ALA:O	3:C:117:ALA:N	2.52	0.42
3:C:132:TRP:NE1	3:C:144:PRO:CD	2.82	0.42
1:E:45:GLN:NE2	1:E:158:ILE:HD11	2.34	0.42
1:E:135:LEU:HD12	1:E:136:LYS:N	2.34	0.42
1:E:211:LEU:O	1:E:214:PHE:HB2	2.19	0.42
2:F:138:ILE:O	2:F:142:LEU:HD13	2.18	0.42
1:I:191:GLY:O	1:I:192:ILE:C	2.61	0.42
1:I:209:TRP:CD1	2:J:92:PHE:HA	2.53	0.42
1:I:219:ILE:CD1	1:I:220:ILE:HG13	2.49	0.42
1:I:404:MET:CE	1:I:414:ALA:HB2	2.49	0.42
2:J:87:ASN:OD1	2:J:87:ASN:N	2.51	0.42
2:J:101:LEU:HD12	2:J:105:GLU:HG3	2.01	0.42
2:J:216:GLU:O	2:J:218:VAL:N	2.52	0.42
2:J:220:VAL:O	2:J:221:ALA:CB	2.67	0.42
3:K:61:TYR:HE2	5:O:2:UNK:N	2.16	0.42
3:K:101:LEU:CD2	4:L:518:UNK:HA	2.49	0.42
1:A:61:TRP:HE1	1:A:74:LEU:CD2	2.32	0.42
1:A:79:HIS:HE1	1:A:416:GLU:OE2	2.02	0.42
1:A:303:VAL:HG12	1:A:304:TYR:N	2.34	0.42
3:C:100:GLU:C	3:C:102:ARG:N	2.72	0.42
1:E:271:LEU:C	1:E:272:GLN:OE1	2.62	0.42
2:F:225:SER:C	4:H:508:UNK:CB	2.93	0.42
3:G:19:VAL:HA	3:G:102:ARG:CD	2.45	0.42
3:G:65:ILE:HD13	5:N:7:UNK:CA	2.49	0.42
3:G:115:ALA:O	3:G:117:ALA:N	2.52	0.42
1:I:48:PHE:CE2	1:I:49:LEU:HD23	2.54	0.42
1:I:61:TRP:CZ2	1:I:161:GLY:HA2	2.53	0.42
1:I:74:LEU:CD1	1:I:147:ALA:HB2	2.49	0.42
1:I:211:LEU:O	1:I:214:PHE:HB2	2.19	0.42
1:I:232:GLU:C	1:I:234:GLN:N	2.76	0.42
1:I:352:TYR:OH	1:I:385:ILE:HG22	2.19	0.42
1:I:385:ILE:HG13	1:I:385:ILE:H	1.56	0.42
2:J:81:GLN:OE1	2:J:94:ALA:HB2	2.19	0.42
2:J:223:PHE:HB3	2:J:224:PHE:H	1.59	0.42
3:K:69:GLU:HB3	3:K:152:MET:HE3	1.98	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:83:TRP:CD1	3:K:87:THR:HG21	2.55	0.42
3:K:89:ASP:CG	3:K:92:VAL:HA	2.43	0.42
3:K:96:ALA:C	3:K:98:ARG:H	2.27	0.42
1:A:110:GLN:CB	1:A:133:ILE:HG22	2.50	0.42
1:A:135:LEU:HD12	1:A:136:LYS:N	2.35	0.42
1:A:191:GLY:O	1:A:194:ARG:HB3	2.20	0.42
1:A:219:ILE:CD1	1:A:220:ILE:HG13	2.49	0.42
1:A:313:ILE:HG22	1:A:314:GLN:H	1.83	0.42
1:A:367:ALA:HB1	1:A:368:PRO:HD2	2.00	0.42
2:B:111:CYS:O	2:B:115:GLY:N	2.49	0.42
3:C:96:ALA:C	3:C:98:ARG:H	2.27	0.42
5:M:2:UNK:O	5:M:6:UNK:N	2.52	0.42
1:E:84:TRP:HB3	1:I:277:LYS:HE3	2.00	0.42
1:E:191:GLY:O	1:E:194:ARG:HB3	2.20	0.42
1:E:352:TYR:OH	1:E:385:ILE:HG22	2.20	0.42
2:F:128:ALA:C	2:F:129:LEU:HG	2.43	0.42
2:F:220:VAL:O	2:F:221:ALA:CB	2.67	0.42
1:I:367:ALA:HB1	1:I:368:PRO:HD2	2.00	0.42
1:I:406:PHE:CE1	1:I:412:ARG:HG2	2.54	0.42
2:J:71:ILE:HD11	2:J:238:PHE:CE1	2.55	0.42
2:J:155:LEU:O	2:J:159:LEU:HD12	2.19	0.42
1:A:352:TYR:OH	1:A:385:ILE:HG22	2.20	0.42
1:A:361:THR:CG2	1:A:362:ASP:N	2.76	0.42
1:A:393:TYR:O	1:E:270:PRO:HG3	2.20	0.42
1:A:406:PHE:CE1	1:A:412:ARG:HG2	2.53	0.42
2:B:140:MET:HG2	2:B:149:THR:HG21	2.01	0.42
1:E:68:VAL:CG1	1:E:173:PHE:H	2.32	0.42
1:E:195:ILE:O	1:E:196:TYR:C	2.63	0.42
1:E:222:SER:HA	1:E:225:ARG:CB	2.47	0.42
1:E:223:TYR:C	1:E:223:TYR:HD1	2.25	0.42
1:E:377:LYS:HE2	1:E:379:GLN:HB2	2.02	0.42
2:F:18:GLU:C	2:F:21:GLY:H	2.27	0.42
2:F:81:GLN:OE1	2:F:94:ALA:HB2	2.19	0.42
2:F:118:TYR:CD1	2:F:118:TYR:N	2.87	0.42
2:F:155:LEU:O	2:F:159:LEU:HD12	2.19	0.42
1:I:53:THR:O	1:I:84:TRP:CZ3	2.73	0.42
1:I:61:TRP:HE1	1:I:74:LEU:CD2	2.32	0.42
1:I:68:VAL:CG1	1:I:173:PHE:H	2.32	0.42
1:I:74:LEU:CG	1:I:147:ALA:HB2	2.48	0.42
1:I:105:LEU:CD1	1:I:135:LEU:HD13	2.45	0.42
1:I:123:LEU:HD21	1:I:149:ILE:HG21	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:200:PHE:CB	1:I:201:PRO:HD3	2.35	0.42
1:I:407:SER:HB3	1:I:411:LYS:H	1.84	0.42
2:J:80:ALA:O	2:J:83:PHE:HB3	2.19	0.42
3:K:113:VAL:O	3:K:114:TYR:C	2.63	0.42
1:A:169:ASP:O	1:A:170:MET:C	2.61	0.42
1:A:261:THR:HG22	1:A:261:THR:O	2.20	0.42
1:A:271:LEU:C	1:A:272:GLN:OE1	2.62	0.42
1:A:339:ASN:O	1:A:342:VAL:HG22	2.20	0.42
2:B:156:GLY:O	2:B:158:GLY:N	2.53	0.42
2:B:204:MET:CA	2:B:206:GLU:OE2	2.67	0.42
2:B:220:VAL:O	2:B:221:ALA:CB	2.67	0.42
3:C:42:GLU:HA	3:C:62:TRP:HZ3	1.81	0.42
1:E:62:SER:HB3	1:E:72:MET:CG	2.50	0.42
1:E:105:LEU:CD2	1:E:166:ILE:HD11	2.50	0.42
1:E:219:ILE:CD1	1:E:220:ILE:HG13	2.49	0.42
1:E:269:ILE:HG13	2:F:184:SER:OG	2.19	0.42
1:E:339:ASN:O	1:E:342:VAL:HG22	2.20	0.42
1:I:247:LEU:C	1:I:247:LEU:CD1	2.90	0.42
2:J:18:GLU:C	2:J:21:GLY:H	2.28	0.42
2:J:73:GLY:O	2:J:157:TRP:CZ2	2.73	0.42
2:J:93:GLY:O	2:J:94:ALA:C	2.61	0.42
2:J:110:TYR:HB3	2:J:111:CYS:H	1.31	0.42
2:J:204:MET:CA	2:J:206:GLU:OE2	2.67	0.42
3:K:65:ILE:HD13	5:O:7:UNK:CA	2.49	0.42
3:K:167:TYR:HD1	3:K:168:ALA:N	2.17	0.42
1:A:53:THR:O	1:A:84:TRP:CZ3	2.73	0.42
1:A:152:GLU:O	1:A:154:GLY:N	2.48	0.42
1:A:269:ILE:HG13	2:B:184:SER:OG	2.19	0.42
1:A:366:LEU:HD12	1:A:370:GLU:CD	2.43	0.42
3:C:85:TRP:O	3:C:88:ARG:HB3	2.19	0.42
3:C:113:VAL:C	3:C:115:ALA:N	2.74	0.42
3:C:127:GLU:O	3:C:127:GLU:HG2	2.20	0.42
1:E:42:GLU:HA	1:E:45:GLN:CG	2.47	0.42
2:F:15:SER:C	2:F:17:ALA:H	2.26	0.42
2:F:44:ILE:HG12	3:G:126:THR:CG2	2.46	0.42
2:F:146:TYR:CZ	2:F:231:MET:CE	3.02	0.42
2:F:156:GLY:O	2:F:158:GLY:N	2.53	0.42
3:G:113:VAL:C	3:G:115:ALA:N	2.75	0.42
1:I:163:TRP:CD1	1:I:163:TRP:N	2.86	0.42
1:I:170:MET:C	1:I:172:ASP:N	2.78	0.42
1:I:261:THR:HG22	1:I:261:THR:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:305:LYS:CE	1:I:310:GLU:HB2	2.42	0.42
2:J:140:MET:HE2	2:J:140:MET:CA	2.49	0.42
3:K:124:PHE:O	3:K:126:THR:N	2.53	0.42
3:K:125:PHE:HD2	3:K:148:ILE:HB	1.80	0.42
1:A:72:MET:HE1	1:A:164:ILE:HG23	2.02	0.42
1:A:157:ILE:HD12	1:A:157:ILE:N	2.17	0.42
1:A:195:ILE:O	1:A:196:TYR:C	2.63	0.42
2:B:71:ILE:HD11	2:B:238:PHE:CE1	2.55	0.42
2:B:73:GLY:O	2:B:157:TRP:CZ2	2.73	0.42
3:C:65:ILE:HD13	5:M:7:UNK:CA	2.49	0.42
1:E:56:TRP:CE2	1:E:159:GLY:HA3	2.55	0.42
1:E:119:ARG:HD3	1:E:119:ARG:N	2.35	0.42
1:E:303:VAL:HG12	1:E:304:TYR:N	2.34	0.42
1:E:380:ASP:OD1	1:E:381:ALA:N	2.52	0.42
1:E:407:SER:O	1:E:408:PRO:C	2.62	0.42
2:F:40:GLY:C	2:F:42:TYR:H	2.27	0.42
2:F:117:THR:HG21	3:G:135:THR:HG21	2.02	0.42
2:F:204:MET:CA	2:F:206:GLU:OE2	2.67	0.42
3:G:53:SER:HA	3:G:58:PHE:CD1	2.54	0.42
1:I:45:GLN:NE2	1:I:158:ILE:HD11	2.35	0.42
1:I:380:ASP:OD1	1:I:381:ALA:N	2.52	0.42
1:I:400:GLY:C	1:I:417:ILE:HD11	2.45	0.42
2:J:62:ARG:NH1	2:J:249:ILE:HD12	2.34	0.42
2:J:68:VAL:C	2:J:70:PRO:CD	2.93	0.42
2:J:68:VAL:CG1	2:J:72:LEU:HD12	2.49	0.42
2:J:225:SER:C	4:L:508:UNK:CB	2.93	0.42
2:J:233:TYR:CD1	2:J:234:PHE:N	2.88	0.42
3:K:35:TYR:CE2	3:K:156:ILE:HD13	2.55	0.42
3:K:44:ILE:CG2	3:K:45:TYR:H	2.27	0.42
1:A:119:ARG:HD3	1:A:119:ARG:N	2.35	0.42
1:A:136:LYS:HE2	1:A:173:PHE:CE1	2.55	0.42
1:A:280:THR:HA	1:A:281:PRO:HD3	1.90	0.42
2:B:23:VAL:C	2:B:25:THR:N	2.77	0.42
2:B:103:ILE:O	2:B:107:ILE:HD12	2.19	0.42
2:B:143:SER:HB3	2:B:148:ILE:CD1	2.39	0.42
2:B:237:TRP:CE3	2:B:238:PHE:N	2.88	0.42
3:C:124:PHE:O	3:C:126:THR:N	2.53	0.42
3:C:168:ALA:O	3:C:172:ILE:HB	2.19	0.42
1:E:53:THR:O	1:E:84:TRP:CZ3	2.73	0.42
2:F:101:LEU:HD12	2:F:105:GLU:HG3	2.01	0.42
2:F:211:ARG:CZ	3:G:157:TYR:CZ	3.03	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:233:TYR:CD1	2:F:234:PHE:N	2.88	0.42
3:G:34:PHE:CE2	3:G:38:VAL:HG21	2.55	0.42
3:G:45:TYR:CE1	3:G:61:TYR:HB3	2.54	0.42
3:G:89:ASP:CG	3:G:92:VAL:HA	2.43	0.42
1:I:62:SER:HB3	1:I:72:MET:CG	2.49	0.42
1:I:119:ARG:HD3	1:I:119:ARG:N	2.35	0.42
1:I:339:ASN:O	1:I:342:VAL:HG22	2.20	0.42
1:I:366:LEU:HD12	1:I:370:GLU:CD	2.43	0.42
1:I:406:PHE:HA	1:I:412:ARG:HA	2.01	0.42
2:J:140:MET:HG2	2:J:149:THR:HG21	2.01	0.42
1:A:200:PHE:C	1:A:200:PHE:CD2	2.98	0.41
1:A:232:GLU:C	1:A:234:GLN:N	2.76	0.41
2:B:18:GLU:C	2:B:21:GLY:H	2.28	0.41
3:C:35:TYR:CE2	3:C:156:ILE:HD13	2.55	0.41
3:C:83:TRP:CD1	3:C:87:THR:HG21	2.55	0.41
3:C:132:TRP:NE1	3:C:144:PRO:CG	2.83	0.41
1:E:74:LEU:CD1	1:E:147:ALA:HB2	2.49	0.41
1:E:400:GLY:C	1:E:417:ILE:HD11	2.45	0.41
2:F:117:THR:HG21	3:G:135:THR:CG2	2.50	0.41
2:F:172:LEU:H	2:F:172:LEU:CD1	2.32	0.41
3:G:61:TYR:HE2	5:N:2:UNK:N	2.16	0.41
3:G:80:LEU:HB3	3:G:84:LEU:HD12	2.02	0.41
3:G:100:GLU:OE1	3:G:173:PRO:HG3	2.19	0.41
4:H:511:UNK:O	4:H:515:UNK:CB	2.68	0.41
1:I:45:GLN:HB2	1:I:50:ARG:HD3	2.01	0.41
1:I:72:MET:HE1	1:I:164:ILE:HG23	2.02	0.41
1:I:135:LEU:HD12	1:I:136:LYS:N	2.34	0.41
1:I:200:PHE:O	1:I:202:TRP:N	2.44	0.41
1:I:210:ILE:CA	2:J:92:PHE:CE1	2.93	0.41
1:I:410:GLY:C	1:I:411:LYS:HG3	2.44	0.41
2:J:40:GLY:C	2:J:42:TYR:H	2.27	0.41
2:J:108:ASN:CA	2:J:112:ASN:HD22	2.33	0.41
3:K:168:ALA:O	3:K:172:ILE:HB	2.19	0.41
1:A:62:SER:HB3	1:A:72:MET:CG	2.50	0.41
1:A:243:GLY:C	1:A:245:ILE:N	2.76	0.41
2:B:44:ILE:HD13	2:B:44:ILE:C	2.43	0.41
2:B:87:ASN:OD1	2:B:87:ASN:N	2.51	0.41
2:B:117:THR:HG21	3:C:135:THR:CG2	2.50	0.41
2:B:243:TYR:O	2:B:247:LYS:HE3	2.21	0.41
3:C:104:HIS:O	3:C:108:VAL:N	2.50	0.41
3:C:104:HIS:O	3:C:107:LEU:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:106:VAL:O	3:C:109:GLU:N	2.50	0.41
2:F:80:ALA:O	2:F:83:PHE:HB3	2.19	0.41
2:F:99:SER:O	2:F:103:ILE:N	2.49	0.41
2:F:215:LYS:HD3	3:G:114:TYR:OH	2.20	0.41
2:F:237:TRP:CE3	2:F:238:PHE:N	2.88	0.41
2:F:243:TYR:O	2:F:247:LYS:HE3	2.20	0.41
3:G:35:TYR:CE2	3:G:156:ILE:HD13	2.54	0.41
3:G:42:GLU:HA	3:G:62:TRP:HZ3	1.81	0.41
3:G:62:TRP:HZ2	3:G:144:PRO:CB	2.31	0.41
3:G:104:HIS:O	3:G:107:LEU:N	2.53	0.41
1:I:110:GLN:CB	1:I:133:ILE:HG22	2.50	0.41
2:J:23:VAL:C	2:J:25:THR:N	2.77	0.41
2:J:237:TRP:CE3	2:J:238:PHE:N	2.88	0.41
3:K:34:PHE:CE2	3:K:38:VAL:HG21	2.55	0.41
3:K:115:ALA:O	3:K:117:ALA:N	2.52	0.41
1:A:119:ARG:NH2	1:I:396:ASP:OD2	2.53	0.41
1:A:173:PHE:HE2	1:A:188:GLU:HG3	1.83	0.41
1:A:400:GLY:C	1:A:417:ILE:HD11	2.45	0.41
1:A:410:GLY:C	1:A:411:LYS:HG3	2.44	0.41
2:B:46:PHE:CE2	2:B:101:LEU:HD21	2.55	0.41
2:B:120:PRO:CD	2:B:123:LEU:HD22	2.41	0.41
3:C:41:TYR:CE1	3:C:62:TRP:CZ3	3.07	0.41
3:C:82:GLY:O	3:C:83:TRP:C	2.63	0.41
1:E:48:PHE:CE2	1:E:49:LEU:HD23	2.54	0.41
1:E:86:GLN:HG3	1:E:87:ALA:N	2.32	0.41
1:E:136:LYS:HE2	1:E:173:PHE:CE1	2.55	0.41
1:E:190:TYR:HD2	1:E:191:GLY:N	2.17	0.41
1:E:232:GLU:C	1:E:234:GLN:N	2.76	0.41
1:E:237:ASP:CA	1:E:240:ARG:HG2	2.46	0.41
1:E:307:PRO:CG	1:E:308:GLY:N	2.80	0.41
1:E:425:PHE:CG	1:I:267:ARG:HD2	2.56	0.41
2:F:46:PHE:CE2	2:F:101:LEU:HD21	2.55	0.41
2:F:103:ILE:O	2:F:107:ILE:HD12	2.19	0.41
1:I:48:PHE:HB3	1:I:394:ASP:HB3	2.00	0.41
1:I:85:PRO:O	1:I:86:GLN:C	2.63	0.41
1:I:191:GLY:O	1:I:194:ARG:HB3	2.20	0.41
1:I:254:THR:C	1:I:256:ILE:N	2.75	0.41
1:I:398:GLN:HG2	1:I:420:PRO:HG3	2.03	0.41
2:J:46:PHE:CE2	2:J:101:LEU:HD21	2.55	0.41
2:J:136:LEU:C	2:J:138:ILE:H	2.28	0.41
2:J:156:GLY:O	2:J:158:GLY:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:195:ARG:HB2	2:J:196:THR:H	1.51	0.41
2:J:215:LYS:HD3	3:K:114:TYR:OH	2.20	0.41
2:J:243:TYR:O	2:J:247:LYS:HE3	2.21	0.41
3:K:80:LEU:HB3	3:K:84:LEU:HD12	2.02	0.41
3:K:104:HIS:O	3:K:107:LEU:N	2.53	0.41
1:A:170:MET:C	1:A:172:ASP:N	2.78	0.41
2:B:76:PHE:O	2:B:80:ALA:CB	2.69	0.41
2:B:98:VAL:O	2:B:100:GLY:N	2.53	0.41
2:B:169:ILE:HG22	2:B:170:ALA:N	2.34	0.41
2:B:215:LYS:HD3	3:C:114:TYR:OH	2.20	0.41
1:E:110:GLN:CB	1:E:133:ILE:HG22	2.50	0.41
1:E:225:ARG:CZ	1:E:233:GLU:HB3	2.51	0.41
1:E:240:ARG:HG3	1:E:241:ARG:N	2.36	0.41
1:E:243:GLY:C	1:E:245:ILE:N	2.76	0.41
2:F:57:VAL:HA	2:F:60:LYS:HG2	2.02	0.41
2:F:71:ILE:HD11	2:F:238:PHE:CE1	2.55	0.41
2:F:102:LEU:N	2:F:102:LEU:CD1	2.84	0.41
2:F:140:MET:HG2	2:F:149:THR:HG21	2.01	0.41
2:F:199:PRO:HD3	3:G:133:HIS:ND1	2.36	0.41
3:G:83:TRP:CD1	3:G:87:THR:HG21	2.55	0.41
3:G:110:TRP:O	3:G:113:VAL:N	2.53	0.41
3:G:124:PHE:HB3	3:G:125:PHE:H	1.70	0.41
3:G:127:GLU:O	3:G:127:GLU:HG2	2.20	0.41
1:I:104:VAL:HG11	1:I:143:TRP:NE1	2.34	0.41
1:I:105:LEU:CD2	1:I:166:ILE:HD11	2.50	0.41
1:I:305:LYS:CG	1:I:310:GLU:H	2.22	0.41
1:I:377:LYS:HE2	1:I:379:GLN:HB2	2.02	0.41
3:K:42:GLU:HA	3:K:62:TRP:HZ3	1.81	0.41
3:K:100:GLU:O	3:K:103:ARG:N	2.50	0.41
1:A:85:PRO:O	1:A:86:GLN:C	2.63	0.41
1:A:156:PRO:O	1:A:156:PRO:CG	2.68	0.41
1:A:380:ASP:OD1	1:A:381:ALA:N	2.52	0.41
2:B:165:ASN:O	2:B:166:TRP:C	2.63	0.41
3:C:55:ALA:O	3:C:58:PHE:HB3	2.21	0.41
3:C:89:ASP:CG	3:C:92:VAL:HA	2.43	0.41
1:E:155:GLY:HA2	1:E:156:PRO:HD3	1.86	0.41
1:E:200:PHE:C	1:E:200:PHE:CD2	2.98	0.41
1:E:305:LYS:CE	1:E:310:GLU:HB2	2.42	0.41
1:E:406:PHE:HA	1:E:412:ARG:HA	2.01	0.41
2:F:23:VAL:C	2:F:25:THR:N	2.77	0.41
2:F:45:HIS:O	2:F:46:PHE:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:73:GLY:O	2:F:157:TRP:CZ2	2.73	0.41
2:F:87:ASN:OD1	2:F:87:ASN:N	2.51	0.41
2:F:91:PRO:O	2:F:137:ASP:OD1	2.38	0.41
2:F:205:VAL:HA	2:J:239:VAL:CG1	2.50	0.41
2:F:228:VAL:C	2:F:230:MET:N	2.64	0.41
3:G:118:ILE:O	3:G:120:TRP:N	2.54	0.41
3:G:132:TRP:NE1	3:G:144:PRO:CD	2.82	0.41
1:I:96:LEU:HG	1:I:110:GLN:NE2	2.36	0.41
1:I:139:ARG:NE	2:J:118:TYR:HE1	2.19	0.41
1:I:150:ASN:HD21	1:I:156:PRO:HB2	1.85	0.41
2:J:30:PHE:O	2:J:31:LEU:C	2.64	0.41
2:J:117:THR:HG21	3:K:135:THR:HG21	2.02	0.41
3:K:76:SER:CB	3:K:159:ILE:HD13	2.49	0.41
1:A:68:VAL:CG1	1:A:173:PHE:H	2.32	0.41
1:A:377:LYS:HE2	1:A:379:GLN:HB2	2.02	0.41
2:B:68:VAL:C	2:B:70:PRO:CD	2.93	0.41
2:B:85:TRP:O	2:B:89:LYS:N	2.54	0.41
3:C:143:THR:HB	3:C:144:PRO:CD	2.41	0.41
3:C:175:PHE:N	3:C:175:PHE:CD2	2.87	0.41
4:D:511:UNK:O	4:D:515:UNK:CB	2.68	0.41
1:E:169:ASP:O	1:E:170:MET:C	2.61	0.41
1:E:261:THR:HG22	1:E:261:THR:O	2.20	0.41
1:E:264:THR:CG2	2:F:171:ALA:HB2	2.51	0.41
2:F:46:PHE:CZ	2:F:69:VAL:HG13	2.56	0.41
2:F:68:VAL:C	2:F:70:PRO:CD	2.93	0.41
3:G:113:VAL:O	3:G:114:TYR:C	2.63	0.41
3:G:132:TRP:NE1	3:G:144:PRO:CG	2.83	0.41
2:J:69:VAL:O	2:J:70:PRO:C	2.61	0.41
2:J:199:PRO:HD3	3:K:133:HIS:ND1	2.36	0.41
2:J:211:ARG:CZ	3:K:157:TYR:CZ	3.03	0.41
3:K:132:TRP:NE1	3:K:144:PRO:CG	2.83	0.41
1:A:74:LEU:CG	1:A:147:ALA:HB2	2.48	0.41
1:A:222:SER:OG	1:A:234:GLN:NE2	2.54	0.41
1:A:264:THR:CG2	2:B:171:ALA:HB2	2.51	0.41
2:B:95:THR:HA	2:B:133:ALA:HB1	2.03	0.41
3:C:24:MET:O	3:C:25:TRP:C	2.61	0.41
3:C:113:VAL:O	3:C:114:TYR:C	2.63	0.41
3:C:159:ILE:HA	3:C:162:VAL:CG2	2.50	0.41
1:E:61:TRP:HE1	1:E:74:LEU:CD2	2.32	0.41
1:E:178:THR:HG23	1:E:182:GLY:C	2.46	0.41
1:E:203:MET:HE2	2:F:103:ILE:HG12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:258:TYR:HD1	2:F:166:TRP:CD1	2.39	0.41
1:E:374:ILE:CD1	1:E:375:GLU:O	2.69	0.41
2:F:98:VAL:O	2:F:100:GLY:N	2.53	0.41
3:G:82:GLY:O	3:G:83:TRP:C	2.63	0.41
3:G:124:PHE:O	3:G:126:THR:N	2.53	0.41
1:I:56:TRP:CE2	1:I:159:GLY:HA3	2.55	0.41
1:I:169:ASP:O	1:I:170:MET:C	2.61	0.41
1:I:200:PHE:C	1:I:200:PHE:CD2	2.98	0.41
1:I:317:VAL:HG23	1:I:374:ILE:HG21	2.03	0.41
1:I:374:ILE:CD1	1:I:375:GLU:O	2.69	0.41
2:J:39:LEU:C	2:J:39:LEU:CD2	2.94	0.41
2:J:117:THR:HG21	3:K:135:THR:CG2	2.50	0.41
2:J:211:ARG:HH11	3:K:154:TYR:HA	1.86	0.41
1:A:105:LEU:CD2	1:A:166:ILE:HD11	2.50	0.41
1:A:110:GLN:CA	1:A:133:ILE:HG22	2.51	0.41
1:A:139:ARG:NE	2:B:118:TYR:HE1	2.19	0.41
2:B:211:ARG:CZ	3:C:157:TYR:CZ	3.03	0.41
3:C:61:TYR:O	3:C:62:TRP:HB2	2.21	0.41
3:C:167:TYR:CD1	3:C:168:ALA:N	2.89	0.41
2:F:175:ALA:HB1	2:F:182:LEU:CD1	2.43	0.41
1:I:138:ARG:HG3	1:I:173:PHE:CD2	2.56	0.41
1:I:157:ILE:H	1:I:157:ILE:CD1	2.13	0.41
1:I:243:GLY:C	1:I:245:ILE:N	2.76	0.41
1:I:328:GLY:O	1:I:329:GLU:HB2	2.21	0.41
1:I:360:SER:HB2	1:I:377:LYS:HB3	2.03	0.41
2:J:46:PHE:CZ	2:J:69:VAL:HG13	2.56	0.41
2:J:76:PHE:O	2:J:80:ALA:CB	2.69	0.41
2:J:103:ILE:O	2:J:107:ILE:CG1	2.69	0.41
2:J:238:PHE:HD1	2:J:241:LYS:CB	2.31	0.41
3:K:45:TYR:CE1	3:K:61:TYR:HB3	2.54	0.41
3:K:55:ALA:O	3:K:58:PHE:HB3	2.21	0.41
3:K:76:SER:O	3:K:79:ALA:HB3	2.21	0.41
3:K:93:ASP:CG	3:K:94:ALA:H	2.29	0.41
3:K:167:TYR:CD1	3:K:168:ALA:N	2.89	0.41
1:A:74:LEU:O	1:A:132:SER:CA	2.68	0.41
1:A:195:ILE:C	1:A:197:ALA:N	2.76	0.41
1:A:258:TYR:HD1	2:B:166:TRP:CD1	2.39	0.41
1:A:374:ILE:CD1	1:A:375:GLU:O	2.69	0.41
2:B:45:HIS:O	2:B:46:PHE:C	2.63	0.41
2:B:102:LEU:N	2:B:102:LEU:CD1	2.84	0.41
2:B:108:ASN:CA	2:B:112:ASN:HD22	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:34:PHE:CE2	3:C:38:VAL:HG21	2.55	0.41
3:C:50:GLY:CA	3:C:58:PHE:HD2	2.31	0.41
3:C:76:SER:O	3:C:79:ALA:HB3	2.21	0.41
3:C:96:ALA:HA	3:C:97:PRO:HD2	1.95	0.41
3:C:110:TRP:O	3:C:113:VAL:N	2.54	0.41
1:E:60:LYS:C	1:E:61:TRP:CE3	2.99	0.41
1:E:150:ASN:HD21	1:E:156:PRO:HB2	1.85	0.41
2:F:85:TRP:O	2:F:89:LYS:N	2.54	0.41
2:F:159:LEU:HG	2:F:247:LYS:HZ3	1.86	0.41
2:F:184:SER:O	2:F:187:ASP:N	2.54	0.41
2:F:199:PRO:CD	3:G:133:HIS:ND1	2.84	0.41
2:F:210:LEU:O	2:F:211:ARG:C	2.64	0.41
2:F:211:ARG:HH11	3:G:154:TYR:HA	1.86	0.41
3:G:31:LEU:CD1	3:G:35:TYR:HD1	2.28	0.41
3:G:55:ALA:HB1	3:G:57:GLU:OE2	2.21	0.41
3:G:80:LEU:HD23	3:G:159:ILE:CG2	2.51	0.41
3:G:93:ASP:CG	3:G:94:ALA:H	2.29	0.41
3:G:152:MET:O	3:G:156:ILE:HG13	2.21	0.41
3:G:167:TYR:CD1	3:G:168:ALA:N	2.89	0.41
1:I:195:ILE:O	1:I:196:TYR:C	2.63	0.41
1:I:196:TYR:OH	2:J:110:TYR:HE1	1.97	0.41
1:I:203:MET:HE2	2:J:103:ILE:HG12	2.03	0.41
1:I:364:THR:HG22	1:I:372:LYS:HZ1	1.81	0.41
2:J:91:PRO:O	2:J:137:ASP:OD1	2.38	0.41
2:J:102:LEU:N	2:J:102:LEU:CD1	2.84	0.41
2:J:185:LEU:O	2:J:186:ALA:C	2.64	0.41
2:J:188:LEU:C	2:J:190:GLY:N	2.76	0.41
2:J:199:PRO:CD	3:K:133:HIS:ND1	2.84	0.41
4:L:511:UNK:O	4:L:515:UNK:CB	2.69	0.41
1:A:96:LEU:HG	1:A:110:GLN:NE2	2.36	0.41
1:A:106:VAL:HG21	1:A:173:PHE:HZ	1.86	0.41
1:A:178:THR:HG23	1:A:182:GLY:C	2.46	0.41
1:A:225:ARG:CZ	1:A:233:GLU:HB3	2.51	0.41
1:A:361:THR:CG2	1:A:362:ASP:H	2.15	0.41
2:B:38:VAL:HG12	2:B:39:LEU:H	1.86	0.41
2:B:62:ARG:HB3	2:B:248:VAL:HG22	2.03	0.41
2:B:140:MET:HE2	2:B:140:MET:CA	2.49	0.41
2:B:199:PRO:CD	3:C:133:HIS:ND1	2.84	0.41
3:C:104:HIS:C	3:C:106:VAL:H	2.29	0.41
3:C:118:ILE:O	3:C:120:TRP:N	2.54	0.41
1:E:139:ARG:NE	2:F:118:TYR:HE1	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:76:PHE:O	2:F:80:ALA:CB	2.69	0.41
2:F:82:ALA:HB1	2:F:146:TYR:HH	1.81	0.41
2:F:218:VAL:HG23	2:F:218:VAL:O	2.21	0.41
1:I:110:GLN:CA	1:I:133:ILE:HG22	2.51	0.41
1:I:201:PRO:HA	1:I:204:ILE:HG13	2.03	0.41
2:J:38:VAL:HG12	2:J:39:LEU:H	1.86	0.41
3:K:61:TYR:O	3:K:62:TRP:HB2	2.21	0.41
3:K:118:ILE:O	3:K:120:TRP:N	2.54	0.41
1:A:105:LEU:CD1	1:A:135:LEU:HD22	2.43	0.40
1:A:150:ASN:HD21	1:A:156:PRO:HB2	1.85	0.40
1:A:177:VAL:CG2	1:A:178:THR:H	2.30	0.40
1:A:357:ARG:H	1:A:357:ARG:HG3	1.62	0.40
1:A:417:ILE:HG13	1:A:418:GLY:N	2.36	0.40
2:B:91:PRO:O	2:B:137:ASP:OD1	2.38	0.40
2:B:103:ILE:O	2:B:107:ILE:CG1	2.69	0.40
3:C:80:LEU:HB3	3:C:84:LEU:HD12	2.02	0.40
3:C:89:ASP:O	3:C:90:ARG:HB3	2.22	0.40
3:C:114:TYR:C	3:C:114:TYR:CD2	2.99	0.40
1:E:215:PHE:C	1:E:217:LYS:N	2.79	0.40
1:E:217:LYS:CD	2:F:24:LYS:NZ	2.84	0.40
1:E:340:PRO:C	1:E:342:VAL:N	2.76	0.40
2:F:95:THR:HA	2:F:133:ALA:HB1	2.03	0.40
2:F:233:TYR:C	2:F:235:LEU:N	2.79	0.40
3:G:85:TRP:CD1	3:G:86:LYS:N	2.89	0.40
1:I:63:LYS:CG	1:I:64:THR:N	2.82	0.40
1:I:417:ILE:HG13	1:I:418:GLY:N	2.36	0.40
2:J:45:HIS:O	2:J:46:PHE:C	2.63	0.40
2:J:98:VAL:O	2:J:100:GLY:N	2.53	0.40
2:J:210:LEU:O	2:J:211:ARG:C	2.64	0.40
2:J:233:TYR:C	2:J:235:LEU:N	2.79	0.40
1:A:105:LEU:HD13	1:A:135:LEU:CD1	2.45	0.40
2:B:57:VAL:HA	2:B:60:LYS:HG2	2.03	0.40
2:B:81:GLN:HE22	2:B:149:THR:HG21	1.86	0.40
2:B:199:PRO:HD3	3:C:133:HIS:ND1	2.36	0.40
3:C:69:GLU:HB2	3:C:152:MET:CE	2.42	0.40
3:C:107:LEU:C	3:C:109:GLU:N	2.76	0.40
3:C:124:PHE:HB3	3:C:125:PHE:H	1.70	0.40
3:C:148:ILE:HA	3:C:152:MET:CB	2.42	0.40
3:C:160:MET:HE2	3:C:160:MET:HB3	1.98	0.40
1:E:49:LEU:O	1:E:50:ARG:C	2.64	0.40
1:E:207:ALA:C	1:E:209:TRP:N	2.79	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:365:PRO:O	1:E:372:LYS:NZ	2.54	0.40
1:E:407:SER:HB3	1:E:411:LYS:H	1.85	0.40
2:F:38:VAL:HG12	2:F:39:LEU:H	1.86	0.40
2:F:69:VAL:O	2:F:70:PRO:C	2.61	0.40
3:G:165:PHE:HD2	3:G:166:PHE:N	2.18	0.40
1:I:42:GLU:HB2	1:I:43:LYS:H	1.66	0.40
1:I:178:THR:HG23	1:I:182:GLY:C	2.46	0.40
1:I:207:ALA:C	1:I:209:TRP:N	2.79	0.40
2:J:81:GLN:HE22	2:J:149:THR:HG21	1.86	0.40
1:A:96:LEU:HD23	1:A:96:LEU:O	2.22	0.40
1:A:163:TRP:CD1	1:A:163:TRP:N	2.86	0.40
1:A:195:ILE:O	1:A:197:ALA:N	2.54	0.40
1:A:342:VAL:HG23	1:A:343:PHE:CD1	2.57	0.40
2:B:46:PHE:CZ	2:B:69:VAL:HG13	2.56	0.40
2:B:68:VAL:HG13	2:B:72:LEU:HD12	2.04	0.40
2:B:176:THR:CG2	2:B:177:GLU:N	2.81	0.40
2:B:223:PHE:HB3	2:B:224:PHE:H	1.59	0.40
3:C:62:TRP:O	3:C:64:SER:N	2.54	0.40
1:E:72:MET:HE1	1:E:164:ILE:HG23	2.02	0.40
1:E:271:LEU:HD23	1:E:271:LEU:N	2.31	0.40
1:E:305:LYS:HB3	1:E:308:GLY:HA3	2.03	0.40
2:F:62:ARG:HB3	2:F:248:VAL:HG22	2.03	0.40
2:F:123:LEU:HD23	2:F:124:VAL:N	2.32	0.40
2:F:136:LEU:C	2:F:138:ILE:H	2.28	0.40
2:F:146:TYR:O	2:F:149:THR:N	2.54	0.40
3:G:159:ILE:O	3:G:162:VAL:CG2	2.64	0.40
3:G:173:PRO:HG2	3:G:174:TYR:N	2.33	0.40
1:I:60:LYS:C	1:I:61:TRP:CE3	2.99	0.40
1:I:135:LEU:O	1:I:136:LYS:HB2	2.22	0.40
1:I:136:LYS:HE2	1:I:173:PHE:CE1	2.55	0.40
1:I:176:PRO:O	1:I:177:VAL:HB	2.22	0.40
1:I:209:TRP:O	1:I:213:TRP:HB2	2.21	0.40
2:J:138:ILE:HG23	2:J:142:LEU:CD1	2.52	0.40
2:J:184:SER:O	2:J:187:ASP:N	2.54	0.40
2:J:218:VAL:O	2:J:218:VAL:HG23	2.21	0.40
2:J:232:VAL:O	2:J:235:LEU:HB3	2.22	0.40
3:K:48:ARG:O	3:K:49:ALA:HB2	2.22	0.40
3:K:62:TRP:O	3:K:64:SER:N	2.54	0.40
3:K:127:GLU:O	3:K:127:GLU:HG2	2.20	0.40
1:A:42:GLU:HB2	1:A:43:LYS:H	1.66	0.40
1:A:209:TRP:O	1:A:213:TRP:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:PHE:C	1:A:217:LYS:N	2.79	0.40
1:A:316:LYS:HD3	1:A:373:THR:HG23	2.03	0.40
1:A:353:LEU:HD12	1:A:353:LEU:N	2.37	0.40
1:A:360:SER:HB2	1:A:377:LYS:HB3	2.03	0.40
1:A:365:PRO:O	1:A:372:LYS:NZ	2.54	0.40
1:A:422:ILE:HG12	2:F:177:GLU:HG3	2.02	0.40
2:B:146:TYR:O	2:B:149:THR:N	2.54	0.40
1:E:96:LEU:HD23	1:E:96:LEU:O	2.22	0.40
1:E:156:PRO:O	1:E:156:PRO:CG	2.68	0.40
1:E:329:GLU:CG	1:E:330:TYR:N	2.80	0.40
1:E:352:TYR:C	1:E:382:ARG:HD3	2.47	0.40
1:E:398:GLN:HG2	1:E:420:PRO:HG3	2.03	0.40
1:E:404:MET:HE2	1:E:414:ALA:HB2	2.04	0.40
2:F:138:ILE:HG23	2:F:142:LEU:CD1	2.52	0.40
3:G:62:TRP:O	3:G:64:SER:N	2.54	0.40
3:G:76:SER:O	3:G:79:ALA:HB3	2.21	0.40
3:G:83:TRP:O	3:G:85:TRP:N	2.55	0.40
1:I:156:PRO:O	1:I:156:PRO:CG	2.68	0.40
1:I:232:GLU:O	1:I:233:GLU:C	2.65	0.40
1:I:352:TYR:C	1:I:382:ARG:HD3	2.47	0.40
2:J:85:TRP:O	2:J:89:LYS:N	2.54	0.40
2:J:146:TYR:O	2:J:149:THR:N	2.54	0.40
3:K:113:VAL:C	3:K:115:ALA:N	2.74	0.40
1:A:305:LYS:CE	1:A:310:GLU:HB2	2.42	0.40
2:B:30:PHE:O	2:B:31:LEU:C	2.64	0.40
2:B:138:ILE:HG23	2:B:142:LEU:CD1	2.52	0.40
2:B:249:ILE:O	2:B:249:ILE:CG2	2.68	0.40
3:C:48:ARG:O	3:C:49:ALA:HB2	2.22	0.40
3:C:85:TRP:CD1	3:C:86:LYS:N	2.89	0.40
1:E:74:LEU:O	1:E:132:SER:CA	2.68	0.40
1:E:209:TRP:O	1:E:213:TRP:HB2	2.21	0.40
1:E:226:ILE:HD13	1:E:226:ILE:HA	1.83	0.40
1:E:239:ASP:O	1:E:242:VAL:HB	2.22	0.40
1:E:279:LEU:HD23	1:E:279:LEU:HA	1.58	0.40
1:E:280:THR:HA	1:E:281:PRO:HD3	1.89	0.40
1:E:356:ASP:O	1:E:358:GLY:N	2.37	0.40
2:F:81:GLN:HE22	2:F:149:THR:HG21	1.86	0.40
3:G:48:ARG:O	3:G:49:ALA:HB2	2.22	0.40
3:G:96:ALA:C	3:G:98:ARG:N	2.76	0.40
1:I:74:LEU:O	1:I:132:SER:CA	2.68	0.40
1:I:119:ARG:HG2	1:I:274:GLY:N	2.24	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:225:ARG:CZ	1:I:233:GLU:HB3	2.51	0.40
1:I:240:ARG:HG3	1:I:241:ARG:N	2.36	0.40
1:I:265:PHE:CD1	1:I:267:ARG:N	2.90	0.40
1:I:361:THR:CG2	1:I:362:ASP:H	2.15	0.40
1:I:404:MET:HE2	1:I:414:ALA:HB2	2.04	0.40
2:J:148:ILE:O	2:J:152:VAL:CG2	2.69	0.40
3:K:83:TRP:O	3:K:85:TRP:N	2.55	0.40
3:K:89:ASP:O	3:K:90:ARG:HB3	2.22	0.40
3:K:124:PHE:HB3	3:K:125:PHE:H	1.70	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:LYS:NZ	1:I:230:LYS:NZ[3_555]	1.64	0.56

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	354/392 (90%)	206 (58%)	86 (24%)	62 (18%)	0	2
1	E	354/392 (90%)	206 (58%)	85 (24%)	63 (18%)	0	2
1	I	354/392 (90%)	206 (58%)	86 (24%)	62 (18%)	0	2
2	B	236/252 (94%)	87 (37%)	74 (31%)	75 (32%)	0	0
2	F	236/252 (94%)	87 (37%)	74 (31%)	75 (32%)	0	0
2	J	236/252 (94%)	87 (37%)	74 (31%)	75 (32%)	0	0
3	C	157/256 (61%)	72 (46%)	51 (32%)	34 (22%)	0	1
3	G	157/256 (61%)	72 (46%)	51 (32%)	34 (22%)	0	1
3	K	157/256 (61%)	72 (46%)	51 (32%)	34 (22%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2241/2700 (83%)	1095 (49%)	632 (28%)	514 (23%)	0 1

All (514) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	42	GLU
1	A	48	PHE
1	A	68	VAL
1	A	81	PHE
1	A	140	ALA
1	A	156	PRO
1	A	173	PHE
1	A	177	VAL
1	A	188	GLU
1	A	195	ILE
1	A	210	ILE
1	A	212	TYR
1	A	217	LYS
1	A	265	PHE
1	A	266	PRO
1	A	279	LEU
1	A	300	LYS
1	A	309	ARG
1	A	374	ILE
1	A	395	THR
2	B	14	HIS
2	B	51	GLY
2	B	71	ILE
2	B	83	PHE
2	B	89	LYS
2	B	98	VAL
2	B	110	TYR
2	B	111	CYS
2	B	112	ASN
2	B	146	TYR
2	B	151	VAL
2	B	155	LEU
2	B	161	PHE
2	B	193	PHE
2	B	201	TYR
2	B	202	ILE
2	B	203	ARG

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Mol	Chain	Res	Type
2	B	210	LEU
2	B	213	PHE
2	B	218	VAL
2	B	219	PRO
2	B	220	VAL
2	B	223	PHE
2	B	239	VAL
2	B	244	SER
3	C	19	VAL
3	C	20	ASP
3	C	44	ILE
3	C	48	ARG
3	C	62	TRP
3	C	92	VAL
3	C	93	ASP
3	C	115	ALA
3	C	138	ARG
3	C	171	ARG
1	E	42	GLU
1	E	48	PHE
1	E	68	VAL
1	E	81	PHE
1	E	140	ALA
1	E	156	PRO
1	E	173	PHE
1	E	177	VAL
1	E	188	GLU
1	E	195	ILE
1	E	210	ILE
1	E	212	TYR
1	E	217	LYS
1	E	265	PHE
1	E	266	PRO
1	E	279	LEU
1	E	300	LYS
1	E	309	ARG
1	E	374	ILE
1	E	395	THR
2	F	14	HIS
2	F	51	GLY
2	F	71	ILE
2	F	83	PHE

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Mol	Chain	Res	Type
2	F	89	LYS
2	F	98	VAL
2	F	110	TYR
2	F	111	CYS
2	F	112	ASN
2	F	146	TYR
2	F	151	VAL
2	F	155	LEU
2	F	161	PHE
2	F	193	PHE
2	F	201	TYR
2	F	202	ILE
2	F	203	ARG
2	F	210	LEU
2	F	213	PHE
2	F	218	VAL
2	F	219	PRO
2	F	220	VAL
2	F	223	PHE
2	F	239	VAL
2	F	244	SER
3	G	19	VAL
3	G	20	ASP
3	G	44	ILE
3	G	48	ARG
3	G	62	TRP
3	G	92	VAL
3	G	93	ASP
3	G	115	ALA
3	G	138	ARG
3	G	171	ARG
1	I	42	GLU
1	I	48	PHE
1	I	68	VAL
1	I	81	PHE
1	I	140	ALA
1	I	156	PRO
1	I	173	PHE
1	I	177	VAL
1	I	188	GLU
1	I	195	ILE
1	I	210	ILE

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Mol	Chain	Res	Type
1	I	212	TYR
1	I	217	LYS
1	I	265	PHE
1	I	266	PRO
1	I	279	LEU
1	I	300	LYS
1	I	309	ARG
1	I	374	ILE
1	I	395	THR
2	J	14	HIS
2	J	51	GLY
2	J	71	ILE
2	J	83	PHE
2	J	89	LYS
2	J	98	VAL
2	J	110	TYR
2	J	111	CYS
2	J	146	TYR
2	J	151	VAL
2	J	155	LEU
2	J	161	PHE
2	J	193	PHE
2	J	201	TYR
2	J	202	ILE
2	J	203	ARG
2	J	210	LEU
2	J	213	PHE
2	J	218	VAL
2	J	219	PRO
2	J	220	VAL
2	J	223	PHE
2	J	239	VAL
2	J	244	SER
3	K	19	VAL
3	K	20	ASP
3	K	44	ILE
3	K	48	ARG
3	K	62	TRP
3	K	92	VAL
3	K	93	ASP
3	K	115	ALA
3	K	138	ARG

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Mol	Chain	Res	Type
3	K	171	ARG
1	A	62	SER
1	A	100	GLU
1	A	106	VAL
1	A	125	VAL
1	A	136	LYS
1	A	171	ALA
1	A	181	ASP
1	A	205	ALA
1	A	228	GLU
1	A	332	ALA
1	A	356	ASP
1	A	358	GLY
1	A	382	ARG
1	A	394	ASP
1	A	417	ILE
2	B	18	GLU
2	B	36	LEU
2	B	46	PHE
2	B	64	MET
2	B	72	LEU
2	B	75	THR
2	B	76	PHE
2	B	86	GLU
2	B	135	TRP
2	B	147	VAL
2	B	170	ALA
2	B	186	ALA
2	B	215	LYS
2	B	221	ALA
2	B	229	SER
2	B	234	PHE
2	B	246	THR
3	C	25	TRP
3	C	27	GLY
3	C	30	GLY
3	C	49	ALA
3	C	86	LYS
3	C	108	VAL
3	C	162	VAL
3	C	173	PRO
1	E	62	SER

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Mol	Chain	Res	Type
1	E	100	GLU
1	E	106	VAL
1	E	125	VAL
1	E	136	LYS
1	E	171	ALA
1	E	181	ASP
1	E	205	ALA
1	E	228	GLU
1	E	332	ALA
1	E	356	ASP
1	E	358	GLY
1	E	382	ARG
1	E	394	ASP
1	E	417	ILE
2	F	18	GLU
2	F	36	LEU
2	F	46	PHE
2	F	64	MET
2	F	72	LEU
2	F	75	THR
2	F	76	PHE
2	F	86	GLU
2	F	135	TRP
2	F	147	VAL
2	F	170	ALA
2	F	186	ALA
2	F	215	LYS
2	F	221	ALA
2	F	229	SER
2	F	234	PHE
2	F	246	THR
3	G	25	TRP
3	G	27	GLY
3	G	30	GLY
3	G	49	ALA
3	G	86	LYS
3	G	108	VAL
3	G	162	VAL
3	G	173	PRO
1	I	62	SER
1	I	100	GLU
1	I	106	VAL

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Mol	Chain	Res	Type
1	I	125	VAL
1	I	136	LYS
1	I	171	ALA
1	I	181	ASP
1	I	205	ALA
1	I	228	GLU
1	I	332	ALA
1	I	356	ASP
1	I	358	GLY
1	I	382	ARG
1	I	394	ASP
1	I	417	ILE
2	J	18	GLU
2	J	36	LEU
2	J	46	PHE
2	J	64	MET
2	J	72	LEU
2	J	75	THR
2	J	76	PHE
2	J	86	GLU
2	J	112	ASN
2	J	135	TRP
2	J	147	VAL
2	J	170	ALA
2	J	186	ALA
2	J	215	LYS
2	J	221	ALA
2	J	229	SER
2	J	234	PHE
2	J	246	THR
3	K	25	TRP
3	K	27	GLY
3	K	30	GLY
3	K	49	ALA
3	K	86	LYS
3	K	108	VAL
3	K	162	VAL
3	K	173	PRO
1	A	47	ALA
1	A	64	THR
1	A	107	ARG
1	A	200	PHE

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Mol	Chain	Res	Type
1	A	235	ILE
1	A	281	PRO
1	A	342	VAL
1	A	363	PRO
1	A	368	PRO
1	A	380	ASP
2	B	22	CYS
2	B	35	PHE
2	B	63	ARG
2	B	106	TRP
2	B	118	TYR
2	B	157	TRP
2	B	167	PRO
2	B	172	LEU
2	B	206	GLU
2	B	240	GLY
3	C	73	GLU
3	C	84	LEU
3	C	90	ARG
3	C	101	LEU
3	C	119	TYR
3	C	125	PHE
3	C	164	ALA
1	E	47	ALA
1	E	64	THR
1	E	107	ARG
1	E	200	PHE
1	E	235	ILE
1	E	281	PRO
1	E	342	VAL
1	E	363	PRO
1	E	368	PRO
1	E	380	ASP
2	F	22	CYS
2	F	35	PHE
2	F	63	ARG
2	F	106	TRP
2	F	118	TYR
2	F	157	TRP
2	F	167	PRO
2	F	172	LEU
2	F	206	GLU

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Mol	Chain	Res	Type
2	F	240	GLY
3	G	73	GLU
3	G	84	LEU
3	G	90	ARG
3	G	101	LEU
3	G	119	TYR
3	G	125	PHE
3	G	164	ALA
1	I	47	ALA
1	I	64	THR
1	I	107	ARG
1	I	200	PHE
1	I	235	ILE
1	I	281	PRO
1	I	342	VAL
1	I	363	PRO
1	I	368	PRO
1	I	380	ASP
2	J	22	CYS
2	J	35	PHE
2	J	63	ARG
2	J	106	TRP
2	J	118	TYR
2	J	157	TRP
2	J	167	PRO
2	J	172	LEU
2	J	206	GLU
2	J	240	GLY
3	K	73	GLU
3	K	84	LEU
3	K	90	ARG
3	K	101	LEU
3	K	119	TYR
3	K	125	PHE
3	K	164	ALA
1	A	189	THR
1	A	208	ALA
1	A	237	ASP
1	A	270	PRO
1	A	307	PRO
1	A	391	LEU
1	A	398	GLN

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Mol	Chain	Res	Type
2	B	23	VAL
2	B	41	GLY
2	B	55	PHE
2	B	66	PRO
2	B	91	PRO
2	B	97	ALA
2	B	99	SER
2	B	131	VAL
2	B	196	THR
2	B	199	PRO
2	B	214	GLY
2	B	217	VAL
3	C	100	GLU
3	C	144	PRO
3	C	174	TYR
1	E	189	THR
1	E	208	ALA
1	E	237	ASP
1	E	270	PRO
1	E	307	PRO
1	E	391	LEU
1	E	398	GLN
2	F	23	VAL
2	F	41	GLY
2	F	55	PHE
2	F	66	PRO
2	F	91	PRO
2	F	97	ALA
2	F	99	SER
2	F	131	VAL
2	F	196	THR
2	F	199	PRO
2	F	214	GLY
2	F	217	VAL
3	G	100	GLU
3	G	144	PRO
3	G	174	TYR
1	I	189	THR
1	I	208	ALA
1	I	237	ASP
1	I	270	PRO
1	I	307	PRO

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Mol	Chain	Res	Type
1	I	391	LEU
1	I	398	GLN
2	J	23	VAL
2	J	41	GLY
2	J	55	PHE
2	J	66	PRO
2	J	91	PRO
2	J	97	ALA
2	J	99	SER
2	J	131	VAL
2	J	196	THR
2	J	199	PRO
2	J	214	GLY
2	J	217	VAL
3	K	100	GLU
3	K	144	PRO
3	K	174	TYR
1	A	46	GLN
1	A	101	PRO
1	A	239	ASP
1	A	393	TYR
1	A	410	GLY
2	B	34	LEU
2	B	47	MET
2	B	65	TRP
2	B	82	ALA
2	B	125	PHE
2	B	211	ARG
2	B	230	MET
3	C	29	ALA
3	C	65	ILE
1	E	46	GLN
1	E	101	PRO
1	E	239	ASP
1	E	393	TYR
1	E	410	GLY
2	F	34	LEU
2	F	47	MET
2	F	65	TRP
2	F	82	ALA
2	F	125	PHE
2	F	211	ARG

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Mol	Chain	Res	Type
2	F	230	MET
3	G	29	ALA
3	G	65	ILE
1	I	46	GLN
1	I	101	PRO
1	I	239	ASP
1	I	393	TYR
1	I	410	GLY
2	J	34	LEU
2	J	47	MET
2	J	65	TRP
2	J	82	ALA
2	J	125	PHE
2	J	211	ARG
2	J	230	MET
3	K	29	ALA
3	K	65	ILE
1	A	278	PRO
2	B	141	LEU
3	C	63	LEU
3	C	116	VAL
1	E	278	PRO
2	F	141	LEU
3	G	63	LEU
3	G	116	VAL
1	I	278	PRO
2	J	141	LEU
3	K	63	LEU
3	K	116	VAL
1	A	91	PRO
2	B	44	ILE
1	E	91	PRO
2	F	44	ILE
1	I	91	PRO
2	J	44	ILE
1	A	201	PRO
1	A	220	ILE
2	B	40	GLY
3	C	28	VAL
3	C	105	VAL
1	E	201	PRO
1	E	220	ILE

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Mol	Chain	Res	Type
2	F	40	GLY
3	G	105	VAL
1	I	201	PRO
1	I	220	ILE
2	J	40	GLY
3	K	28	VAL
3	K	105	VAL
3	G	28	VAL
1	A	219	ILE
1	E	219	ILE
1	I	219	ILE
2	B	93	GLY
1	E	176	PRO
2	F	93	GLY
2	J	93	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	298/322 (92%)	254 (85%)	44 (15%)	3	16
1	E	298/322 (92%)	254 (85%)	44 (15%)	3	16
1	I	298/322 (92%)	254 (85%)	44 (15%)	3	16
2	B	197/207 (95%)	147 (75%)	50 (25%)	0	4
2	F	197/207 (95%)	147 (75%)	50 (25%)	0	4
2	J	197/207 (95%)	147 (75%)	50 (25%)	0	4
3	C	135/208 (65%)	114 (84%)	21 (16%)	2	15
3	G	135/208 (65%)	114 (84%)	21 (16%)	2	15
3	K	135/208 (65%)	114 (84%)	21 (16%)	2	15
All	All	1890/2211 (86%)	1545 (82%)	345 (18%)	2	11

All (345) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	HIS
1	A	42	GLU
1	A	48	PHE
1	A	63	LYS
1	A	73	VAL
1	A	74	LEU
1	A	80	VAL
1	A	86	GLN
1	A	116	PHE
1	A	134	ASP
1	A	135	LEU
1	A	143	TRP
1	A	148	GLN
1	A	152	GLU
1	A	156	PRO
1	A	157	ILE
1	A	179	LEU
1	A	187	LEU
1	A	193	ASP
1	A	196	TYR
1	A	213	TRP
1	A	214	PHE
1	A	226	ILE
1	A	228	GLU
1	A	233	GLU
1	A	268	THR
1	A	275	LEU
1	A	276	GLN
1	A	279	LEU
1	A	283	ILE
1	A	295	VAL
1	A	353	LEU
1	A	354	LEU
1	A	359	LEU
1	A	361	THR
1	A	366	LEU
1	A	374	ILE
1	A	375	GLU
1	A	385	ILE
1	A	393	TYR
1	A	394	ASP
1	A	413	TYR
1	A	422	ILE

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Mol	Chain	Res	Type
1	A	425	PHE
2	B	22	CYS
2	B	29	MET
2	B	32	THR
2	B	33	LEU
2	B	44	ILE
2	B	49	THR
2	B	55	PHE
2	B	59	TRP
2	B	83	PHE
2	B	84	PHE
2	B	87	ASN
2	B	90	LEU
2	B	106	TRP
2	B	114	TRP
2	B	116	TRP
2	B	118	TYR
2	B	121	ILE
2	B	123	LEU
2	B	140	MET
2	B	141	LEU
2	B	142	LEU
2	B	146	TYR
2	B	164	ASN
2	B	166	TRP
2	B	167	PRO
2	B	169	ILE
2	B	188	LEU
2	B	193	PHE
2	B	194	VAL
2	B	195	ARG
2	B	198	MET
2	B	200	GLU
2	B	202	ILE
2	B	206	GLU
2	B	210	LEU
2	B	212	THR
2	B	215	LYS
2	B	217	VAL
2	B	218	VAL
2	B	219	PRO
2	B	224	PHE

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Mol	Chain	Res	Type
2	B	227	PHE
2	B	228	VAL
2	B	232	VAL
2	B	233	TYR
2	B	234	PHE
2	B	237	TRP
2	B	239	VAL
2	B	242	TRP
2	B	245	THR
3	C	33	ILE
3	C	35	TYR
3	C	63	LEU
3	C	65	ILE
3	C	68	THR
3	C	70	ILE
3	C	88	ARG
3	C	90	ARG
3	C	99	GLU
3	C	101	LEU
3	C	102	ARG
3	C	138	ARG
3	C	146	HIS
3	C	147	ILE
3	C	150	PHE
3	C	152	MET
3	C	159	ILE
3	C	165	PHE
3	C	166	PHE
3	C	167	TYR
3	C	170	THR
1	E	40	HIS
1	E	42	GLU
1	E	48	PHE
1	E	63	LYS
1	E	73	VAL
1	E	74	LEU
1	E	80	VAL
1	E	86	GLN
1	E	116	PHE
1	E	134	ASP
1	E	135	LEU
1	E	143	TRP

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Mol	Chain	Res	Type
1	E	148	GLN
1	E	152	GLU
1	E	156	PRO
1	E	157	ILE
1	E	179	LEU
1	E	187	LEU
1	E	193	ASP
1	E	196	TYR
1	E	213	TRP
1	E	214	PHE
1	E	226	ILE
1	E	228	GLU
1	E	233	GLU
1	E	268	THR
1	E	275	LEU
1	E	276	GLN
1	E	279	LEU
1	E	283	ILE
1	E	295	VAL
1	E	353	LEU
1	E	354	LEU
1	E	359	LEU
1	E	361	THR
1	E	366	LEU
1	E	374	ILE
1	E	375	GLU
1	E	385	ILE
1	E	393	TYR
1	E	394	ASP
1	E	413	TYR
1	E	422	ILE
1	E	425	PHE
2	F	22	CYS
2	F	29	MET
2	F	32	THR
2	F	33	LEU
2	F	44	ILE
2	F	49	THR
2	F	55	PHE
2	F	59	TRP
2	F	83	PHE
2	F	84	PHE

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Mol	Chain	Res	Type
2	F	87	ASN
2	F	90	LEU
2	F	106	TRP
2	F	114	TRP
2	F	116	TRP
2	F	118	TYR
2	F	121	ILE
2	F	123	LEU
2	F	140	MET
2	F	141	LEU
2	F	142	LEU
2	F	146	TYR
2	F	164	ASN
2	F	166	TRP
2	F	167	PRO
2	F	169	ILE
2	F	188	LEU
2	F	193	PHE
2	F	194	VAL
2	F	195	ARG
2	F	198	MET
2	F	200	GLU
2	F	202	ILE
2	F	206	GLU
2	F	210	LEU
2	F	212	THR
2	F	215	LYS
2	F	217	VAL
2	F	218	VAL
2	F	219	PRO
2	F	224	PHE
2	F	227	PHE
2	F	228	VAL
2	F	232	VAL
2	F	233	TYR
2	F	234	PHE
2	F	237	TRP
2	F	239	VAL
2	F	242	TRP
2	F	245	THR
3	G	33	ILE
3	G	35	TYR

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Mol	Chain	Res	Type
3	G	63	LEU
3	G	65	ILE
3	G	68	THR
3	G	70	ILE
3	G	88	ARG
3	G	90	ARG
3	G	99	GLU
3	G	101	LEU
3	G	102	ARG
3	G	138	ARG
3	G	146	HIS
3	G	147	ILE
3	G	150	PHE
3	G	152	MET
3	G	159	ILE
3	G	165	PHE
3	G	166	PHE
3	G	167	TYR
3	G	170	THR
1	I	40	HIS
1	I	42	GLU
1	I	48	PHE
1	I	63	LYS
1	I	73	VAL
1	I	74	LEU
1	I	80	VAL
1	I	86	GLN
1	I	116	PHE
1	I	134	ASP
1	I	135	LEU
1	I	143	TRP
1	I	148	GLN
1	I	152	GLU
1	I	156	PRO
1	I	157	ILE
1	I	179	LEU
1	I	187	LEU
1	I	193	ASP
1	I	196	TYR
1	I	213	TRP
1	I	214	PHE
1	I	226	ILE

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Mol	Chain	Res	Type
1	I	228	GLU
1	I	233	GLU
1	I	268	THR
1	I	275	LEU
1	I	276	GLN
1	I	279	LEU
1	I	283	ILE
1	I	295	VAL
1	I	353	LEU
1	I	354	LEU
1	I	359	LEU
1	I	361	THR
1	I	366	LEU
1	I	374	ILE
1	I	375	GLU
1	I	385	ILE
1	I	393	TYR
1	I	394	ASP
1	I	413	TYR
1	I	422	ILE
1	I	425	PHE
2	J	22	CYS
2	J	29	MET
2	J	32	THR
2	J	33	LEU
2	J	44	ILE
2	J	49	THR
2	J	55	PHE
2	J	59	TRP
2	J	83	PHE
2	J	84	PHE
2	J	87	ASN
2	J	90	LEU
2	J	106	TRP
2	J	114	TRP
2	J	116	TRP
2	J	118	TYR
2	J	121	ILE
2	J	123	LEU
2	J	140	MET
2	J	141	LEU
2	J	142	LEU

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Mol	Chain	Res	Type
2	J	146	TYR
2	J	164	ASN
2	J	166	TRP
2	J	167	PRO
2	J	169	ILE
2	J	188	LEU
2	J	193	PHE
2	J	194	VAL
2	J	195	ARG
2	J	198	MET
2	J	200	GLU
2	J	202	ILE
2	J	206	GLU
2	J	210	LEU
2	J	212	THR
2	J	215	LYS
2	J	217	VAL
2	J	218	VAL
2	J	219	PRO
2	J	224	PHE
2	J	227	PHE
2	J	228	VAL
2	J	232	VAL
2	J	233	TYR
2	J	234	PHE
2	J	237	TRP
2	J	239	VAL
2	J	242	TRP
2	J	245	THR
3	K	33	ILE
3	K	35	TYR
3	K	63	LEU
3	K	65	ILE
3	K	68	THR
3	K	70	ILE
3	K	88	ARG
3	K	90	ARG
3	K	99	GLU
3	K	101	LEU
3	K	102	ARG
3	K	138	ARG
3	K	146	HIS

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Mol	Chain	Res	Type
3	K	147	ILE
3	K	150	PHE
3	K	152	MET
3	K	159	ILE
3	K	165	PHE
3	K	166	PHE
3	K	167	TYR
3	K	170	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	GLN
1	A	46	GLN
1	A	55	ASN
1	A	79	HIS
1	A	110	GLN
1	A	150	ASN
1	A	199	HIS
1	A	262	ASN
1	A	314	GLN
1	A	398	GLN
2	B	14	HIS
2	B	108	ASN
2	B	112	ASN
2	B	165	ASN
2	B	174	GLN
2	B	181	GLN
3	C	32	ASN
3	C	91	ASN
3	C	128	GLN
1	E	45	GLN
1	E	46	GLN
1	E	55	ASN
1	E	79	HIS
1	E	110	GLN
1	E	150	ASN
1	E	199	HIS
1	E	262	ASN
1	E	314	GLN
1	E	398	GLN
2	F	14	HIS

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Mol	Chain	Res	Type
2	F	108	ASN
2	F	112	ASN
2	F	165	ASN
2	F	174	GLN
2	F	181	GLN
3	G	32	ASN
3	G	91	ASN
1	I	45	GLN
1	I	46	GLN
1	I	55	ASN
1	I	79	HIS
1	I	110	GLN
1	I	150	ASN
1	I	199	HIS
1	I	262	ASN
1	I	314	GLN
1	I	398	GLN
2	J	14	HIS
2	J	108	ASN
2	J	112	ASN
2	J	165	ASN
2	J	174	GLN
2	J	181	GLN
3	K	32	ASN
3	K	91	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	362/392 (92%)	0.43	25 (6%) 23 20	145, 145, 145, 145	0
1	E	362/392 (92%)	0.34	12 (3%) 49 34	145, 145, 145, 145	0
1	I	362/392 (92%)	0.45	18 (4%) 34 26	145, 145, 145, 145	0
2	B	238/252 (94%)	0.58	18 (7%) 20 19	145, 145, 145, 145	0
2	F	238/252 (94%)	0.73	24 (10%) 12 15	145, 145, 145, 145	0
2	J	238/252 (94%)	0.77	25 (10%) 11 14	145, 145, 145, 145	0
3	C	159/256 (62%)	0.64	13 (8%) 17 18	145, 145, 145, 145	0
3	G	159/256 (62%)	0.69	14 (8%) 15 17	145, 145, 145, 145	0
3	K	159/256 (62%)	0.62	14 (8%) 15 17	145, 145, 145, 145	0
4	D	0/20	-	-	-	-
4	H	0/20	-	-	-	-
4	L	0/20	-	-	-	-
5	M	0/26	-	-	-	-
5	N	0/26	-	-	-	-
5	O	0/26	-	-	-	-
All	All	2277/2838 (80%)	0.55	163 (7%) 21 20	145, 145, 145, 145	0

All (163) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	139	ASP	9.0
2	B	199	PRO	7.6
1	I	82	SER	7.0
1	I	73	VAL	6.5
2	F	197	SER	6.2
2	J	199	PRO	6.0
1	I	134	ASP	5.9
3	K	47	TRP	5.6
3	G	45	TYR	5.4

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Mol	Chain	Res	Type	RSRZ
3	C	164	ALA	5.3
2	B	197	SER	5.3
2	F	13	PHE	5.3
1	I	264	THR	5.0
1	E	235	ILE	4.5
2	J	75	THR	4.5
3	C	139	ASP	4.5
3	K	174	TYR	4.4
3	G	25	TRP	4.4
2	F	58	ASP	4.3
2	F	22	CYS	4.3
2	J	213	PHE	4.3
3	G	58	PHE	4.2
2	J	171	ALA	4.2
2	J	117	THR	4.1
2	F	56	TRP	4.0
3	C	114	TYR	4.0
2	B	193	PHE	3.9
2	J	197	SER	3.8
1	I	353	LEU	3.8
2	F	98	VAL	3.8
2	F	72	LEU	3.8
3	G	53	SER	3.8
1	I	175	ASP	3.7
2	J	114	TRP	3.6
2	J	80	ALA	3.6
2	B	226	GLY	3.5
2	J	198	MET	3.5
1	A	229	GLY	3.4
3	K	34	PHE	3.4
2	J	168	ALA	3.3
3	G	142	PHE	3.3
3	C	93	ASP	3.3
2	J	58	ASP	3.2
1	E	101	PRO	3.2
1	I	406	PHE	3.2
1	E	196	TYR	3.2
1	A	371	THR	3.1
3	C	145	SER	3.1
1	A	73	VAL	3.1
2	J	226	GLY	3.1
3	K	51	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
3	K	50	GLY	3.0
2	J	76	PHE	3.0
1	I	352	TYR	3.0
2	J	118	TYR	3.0
3	C	136	VAL	3.0
1	A	57	TYR	3.0
2	J	87	ASN	3.0
1	I	317	VAL	3.0
3	K	104	HIS	2.9
2	B	122	SER	2.9
2	J	59	TRP	2.9
2	B	120	PRO	2.9
1	A	199	HIS	2.8
2	F	217	VAL	2.8
2	F	49	THR	2.8
1	A	235	ILE	2.8
2	J	120	PRO	2.8
1	E	188	GLU	2.8
2	F	106	TRP	2.8
3	K	83	TRP	2.8
1	E	195	ILE	2.8
1	I	404	MET	2.8
2	B	53	TRP	2.8
2	F	195	ARG	2.8
3	G	52	ASP	2.8
1	I	361	THR	2.8
2	J	63	ARG	2.7
1	A	366	LEU	2.7
1	A	185	VAL	2.7
3	C	160	MET	2.7
2	F	75	THR	2.7
1	A	177	VAL	2.7
1	A	396	ASP	2.7
3	G	85	TRP	2.7
3	K	30	GLY	2.6
3	C	30	GLY	2.6
3	K	54	PHE	2.6
2	F	199	PRO	2.6
1	A	353	LEU	2.6
1	E	400	GLY	2.6
2	J	19	ALA	2.6
1	I	187	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
3	C	111	LEU	2.6
3	G	164	ALA	2.6
2	F	38	VAL	2.5
2	F	76	PHE	2.5
3	K	49	ALA	2.5
2	F	237	TRP	2.5
3	K	116	VAL	2.5
2	B	125	PHE	2.5
3	G	140	THR	2.5
1	A	393	TYR	2.5
3	G	160	MET	2.5
3	C	161	ALA	2.5
1	A	275	LEU	2.5
3	K	136	VAL	2.5
2	F	53	TRP	2.4
2	F	168	ALA	2.4
1	A	96	LEU	2.4
1	E	368	PRO	2.4
2	F	182	LEU	2.4
2	J	147	VAL	2.4
1	A	374	ILE	2.4
2	F	86	GLU	2.4
2	F	19	ALA	2.4
3	K	67	TRP	2.4
2	F	190	GLY	2.4
2	B	223	PHE	2.4
1	A	253	ALA	2.4
2	F	42	TYR	2.4
3	C	154	TYR	2.4
1	A	230	LYS	2.4
1	I	101	PRO	2.3
3	K	26	VAL	2.3
1	A	215	PHE	2.3
1	A	192	ILE	2.3
3	G	18	ILE	2.3
1	E	308	GLY	2.3
2	B	89	LYS	2.2
2	B	38	VAL	2.2
1	A	134	ASP	2.2
1	I	199	HIS	2.2
1	I	83	ALA	2.2
2	J	53	TRP	2.2

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Mol	Chain	Res	Type	RSRZ
1	I	228	GLU	2.2
2	F	101	LEU	2.2
1	E	392	ALA	2.2
2	B	170	ALA	2.2
1	E	272	GLN	2.2
2	J	211	ARG	2.1
2	J	218	VAL	2.1
1	A	182	GLY	2.1
2	B	75	THR	2.1
2	B	210	LEU	2.1
1	I	140	ALA	2.1
3	C	83	TRP	2.1
1	I	311	LEU	2.1
1	A	244	ALA	2.1
1	E	59	VAL	2.1
2	B	233	TYR	2.1
3	C	101	LEU	2.1
3	G	111	LEU	2.1
3	G	28	VAL	2.1
1	A	195	ILE	2.0
2	B	121	ILE	2.0
2	B	126	PRO	2.0
2	B	246	THR	2.0
1	A	58	ASP	2.0
1	E	118	PRO	2.0
2	J	149	THR	2.0
2	J	235	LEU	2.0
1	A	132	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	CU	E	722	1/1	0.89	0.06	127,127,127,127	0
6	CU	I	732	1/1	0.94	0.05	127,127,127,127	0
6	CU	I	731	1/1	0.95	0.05	119,119,119,119	0
6	CU	E	721	1/1	0.95	0.05	119,119,119,119	0
6	CU	G	662	1/1	0.97	0.16	118,118,118,118	0
6	CU	K	663	1/1	0.97	0.04	118,118,118,118	0
6	CU	A	712	1/1	0.98	0.04	127,127,127,127	0
6	CU	C	661	1/1	0.98	0.03	118,118,118,118	0
6	CU	A	711	1/1	0.99	0.05	119,119,119,119	0

6.5 Other polymers [i](#)

There are no such residues in this entry.